ON A COMBINATORIAL GENERATION PROBLEM OF KNUTH

ARTURO MERINO, ONDŘEJ MIČKA, AND TORSTEN MÜTZE

Abstract. The well-known middle levels conjecture asserts that for every integer $n \geq 1$, all binary strings of length $2(n+1)$ with exactly $n+1$ many 0s and 1s can be ordered cyclically so that any two consecutive strings differ in swapping the first bit with a complementary bit at some later position. In his book 'The Art of Computer Programming Vol. 4A' Knuth raised a stronger form of this conjecture (Problem 56 in Section 7.2.1.3), which requires that the sequence of positions with which the first bit is swapped in each step of such an ordering has $2n+1$ blocks of the same length, and each block is obtained by adding $s = 1$ (modulo $2n+1$) to the previous block. In this work, we prove Knuth's conjecture in a more general form, allowing for arbitrary shifts $s \geq 1$ that are coprime to $2n+1$. We also present an algorithm to compute this ordering, generating each new bitstring in $\mathcal{O}(n)$ time, using $\mathcal{O}(n)$ memory in total.

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1. Introduction

In computer science and mathematics we frequently encounter various fundamental classes of combinatorial objects such as subsets, permutations, combinations, partitions, trees etc. There are essentially three recurring algorithmic tasks we want to perform with such objects, namely counting (how many objects are there?), random generation (pick one object uniformly at random), and exhaustive generation (generate every object exactly once). The focus of this paper is on the latter of these tasks, namely algorithms for exhaustively generating a class of combinatorial objects. This research area has flourished tremendously, in particular since the advent of powerful computers, and many of the gems it has produced are treated in depth in the most recent volume of Knuth's seminal series 'The Art of Computer Programming' [Knu11] (see also the classical book by Nijenhuis and Wilf [NW75]).

1.1. Combination generation.

1.1. Combination generation. One of the basic classes of combinatorial objects we want to generate are (k,ℓ)-*combinations*, i.e., all ways of choosing a subset of a fixed size k from the ground set $[n] := \{1,\ldots,n\}$ where $n := k+\ell$. In a computer we conveniently encode every set by a bitstring of length n with exactly k many 1s, where the ith bit is 1 if and only if the element i is contained in the set. For instance, all 2-element subsets of the 4-element ground set $\{1,2,3,4\}$ are 12, 13, 14, 23, 24, 34, where we omit curly brackets and commas for simplicity, and the corresponding bitstrings are $1100, 1010, 1001, 0110, 0101, 0011$. As we are concerned with fast generation algorithms, a natural approach is to generate a class of objects in an order such that any two consecutive objects differ only by a small amount, i.e., we aim for a *Gray code* ordering. In general, a combinatorial Gray code is a minimum change ordering of objects for some specified closeness criterion, and fast algorithms for generating such orderings have been discovered for a large variety of combinatorial objects of interest (see [Sav97, Knu11]). For combinations, we aim for an ordering where any two consecutive sets differ only in exchanging a single element, such as $(12,13,14,24,34,23) = (1\underline{1}\underline{0}0, 10\underline{1}\underline{0}, \underline{1}\underline{0}01, 0\underline{1}\underline{0}1, 0\underline{0}1\underline{1}, \underline{0}1\underline{1}0)$. As we can see, this corresponds to swapping a 0-bit with a 1-bit in the bitstring representation in every step, where the two swapped bits are underlined in the example.

1.2. The middle levels conjecture. In the 1980s, Buck and Wiedemann [BW84] conjectured that all $(n+1,n+1)$-combinations can be generated by *star transpositions* for every $n \geq 1$, i.e., the element 1 either enters or leaves the set in each step. In terms of bitstrings, this means that in every step the first bit is swapped with a complementary bit at a later position. The ordering is also required to be cyclic, i.e., this transition rule must also hold when going from the last combination back to the first. The corresponding *flip sequence* α records the position of the bit with which the first bit is swapped in each step, where positions are indexed by $0,\ldots,2n+1$, so the entries of α are from the set $\{1,\ldots,2n+1\}$ and α has length $N := \binom{2(n+1)}{n+1}$. For example, a cyclic star transposition ordering of $(2,2)$-combinations is $(12,23,13,34,14,24) = (\underline{1}1\underline{0}0, \underline{0}\underline{1}10, \underline{1}01\underline{0}, \underline{0}0\underline{1}1, \underline{1}\underline{0}01, \underline{0}10\underline{1})$, and the corresponding flip sequence is $\alpha = 213213$. Buck and Wiedemann's conjecture was raised independently by Havel [Hav83] and became known as *middle levels conjecture*. The name appeals to the middle two levels of the $(2n+1)$-dimensional hypercube. This conjecture received considerable attention in the literature (see [FT95, SW95, Joh04, HKRR05, GŠ10, KT88, DSW88, DKS94]), as it lies at the heart of several related combinatorial generation problems. It is also mentioned in the popular books by Winkler [Win04] and by Diaconis and Graham [DG12], and in Gowers' survey [Gow17]. Eventually, the middle levels conjecture was solved by Mütze [Müt16] and a simplified proof appeared in [GMN18]. Moreover, a constant-time algorithm for computing a star transposition ordering for $(n+1,n+1)$-combinations for every $n \geq 1$ was presented at SODA 2017 [MN17].

1.3. **Knuth's stronger conjecture.** In Problem 56 in Section 7.2.1.3 of his book [Knu11] (page 735), which was ranked as the hardest open problem in the book with a difficulty rating of 49/50, Knuth raised a stronger version of the middle levels conjecture, which requires additional symmetry in the flip sequence. Specifically, Knuth conjectured that there is a star transposition ordering of $(n+1,n+1)$-combinations for every $n \geq 1$ such that the flip sequence α has a block structure $\alpha = (\alpha_0, \alpha_1, \ldots, \alpha_{2n})$, where each block α_i has the same length $N/(2n+1)$ and is obtained from the initial block α_0 by element-wise addition of i modulo $2n+1$ for all $i = 1, \ldots, 2n$. As the entries of α are from $\{1, \ldots, 2n+1\}$, the numbers $1, \ldots, 2n+1$ are chosen as residue class representatives for this addition, rather than $0, \ldots, 2n$. In other words, such a flip sequence α has cyclic symmetry and the initial block α_0 alone encodes the entire flip sequence α by a factor of $2n+1$ more compactly. The compression factor $2n+1$ is best possible, and it arises from the fact that every bitstring obtained by removing the first bit of an $(n+1,n+1)$-combination has exactly $2n+1$ distinct cyclic rotations. Also note that $N/(2n+1) = 2C_n$, where $C_n := \frac{1}{n+1}\binom{2n}{n}$ is the nth Catalan number. For instance, for $n = 2$ we have $N = 20$, and all $(3,3)$-combinations can be generated from 111000 by the flip sequence (4134 5245 1351 2412 3523), i.e., with initial block $\alpha_0 := 4134$. Similarly, for $n = 3$ we have $N = 70$, and all $(4,4)$-combinations can be generated from 11110000 by the flip sequence defined by the initial block $\alpha_0 := 6253462135$. The entire ordering of combinations obtained for this example is shown in the first column in Figure 1. In fact, the compact encoding of the flip sequence required in Knuth's problem was the main tool researchers used in tackling the middle levels conjecture experimentally, as it allows restricting the search space by a factor of $2n+1$ (which yields an exponential speedup for brute-force searches). This approach was already employed by Buck and Wiedemann [BW84] for $n = 3, 4, 5$, and was later refined and implemented on powerful computers by Shields, Shields, and Savage [SSS09] for values up to $n \leq 17$ and by Shimada and Amano [SA11] for $n = 18, 19$.

1.4. **Our results.** Unfortunately, none of the flip sequences constructed in [Müt16, MN17, GMN18] to solve the middle levels conjecture satisfy the stronger symmetry requirements of Knuth's problem. The main contribution of this work is to solve Knuth's symmetric version of the middle levels conjecture in the following more general form, allowing for arbitrary shifts; see Figure 1 for illustration.

Theorem 1. *For any $n \geq 1$ and $1 \leq s \leq 2n$ that is coprime to $2n+1$, there is a star transposition ordering of all $(n+1,n+1)$-combinations such that the corresponding flip sequence is $\alpha = (\alpha_0, \alpha_1, \ldots, \alpha_{2n})$, and each block α_i is obtained from the initial block α_0 by element-wise addition of $i \cdot s$ modulo $2n+1$ for all $i = 1, \ldots, 2n$.*

In Section 1.6 below we explain why the condition on s to be coprime to $2n+1$ is necessary and cannot be omitted from Theorem 1. Our proof of Theorem 1 is constructive, and translates into an algorithm that generates $(n+1,n+1)$-combinations by star transpositions efficiently.

Theorem 2. *There is an algorithm that computes, for any $n \geq 1$ and $1 \leq s \leq 2n$ that is coprime to $2n+1$, a star transposition ordering of all $(n+1,n+1)$-combinations as in Theorem 1, with running time $\mathcal{O}(n)$ for each generated combination, using $\mathcal{O}(n)$ memory in total.*

The initial combination can be chosen arbitrarily in our algorithm, and the initialization time is $\mathcal{O}(n^2)$. We implemented this algorithm in C++ and made it available for download and experimentation on the Combinatorial Object Server website [cos]. It is open whether our algorithm can be improved to generate each combination in time $\mathcal{O}(1)$ instead of $\mathcal{O}(n)$.

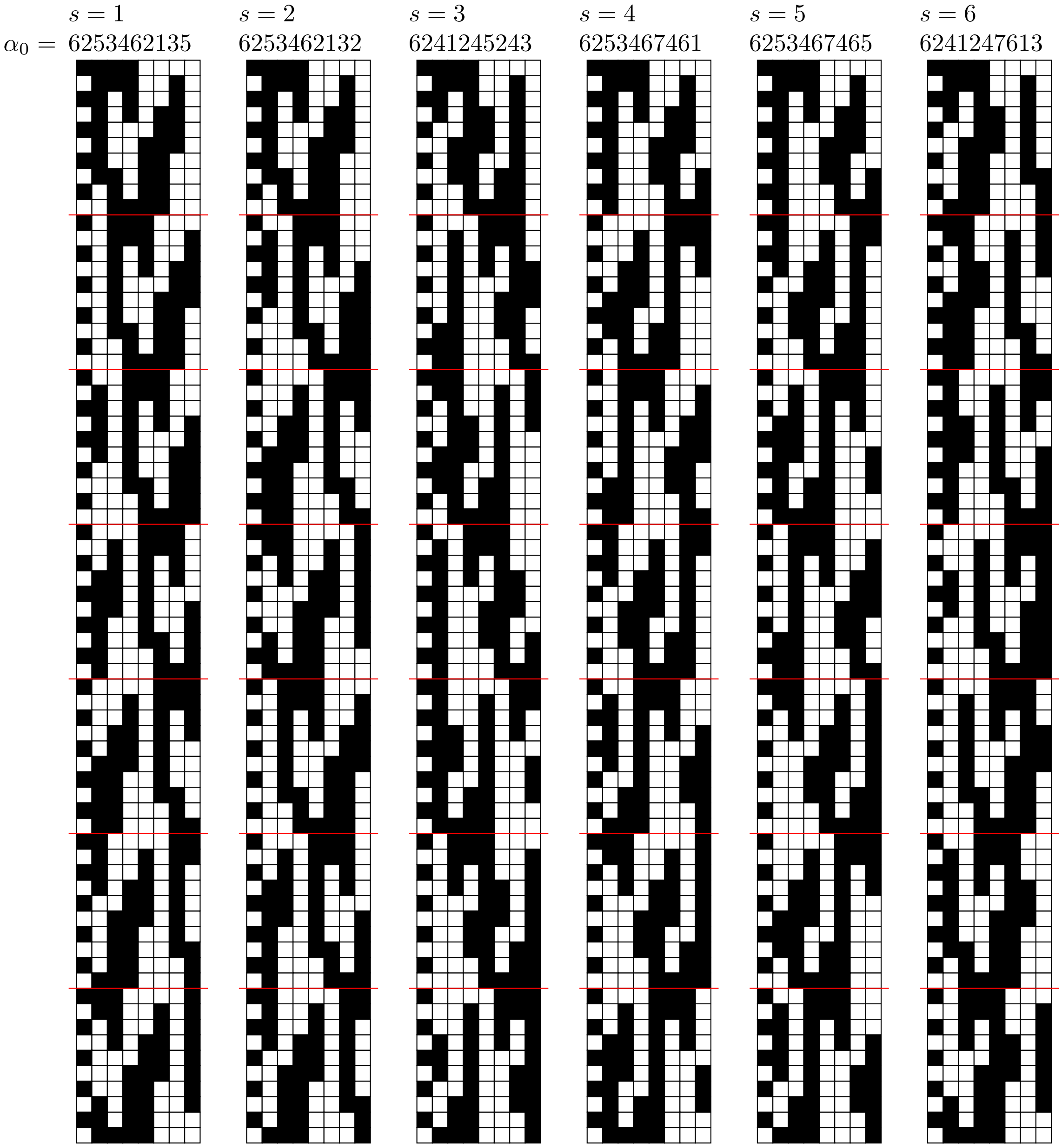
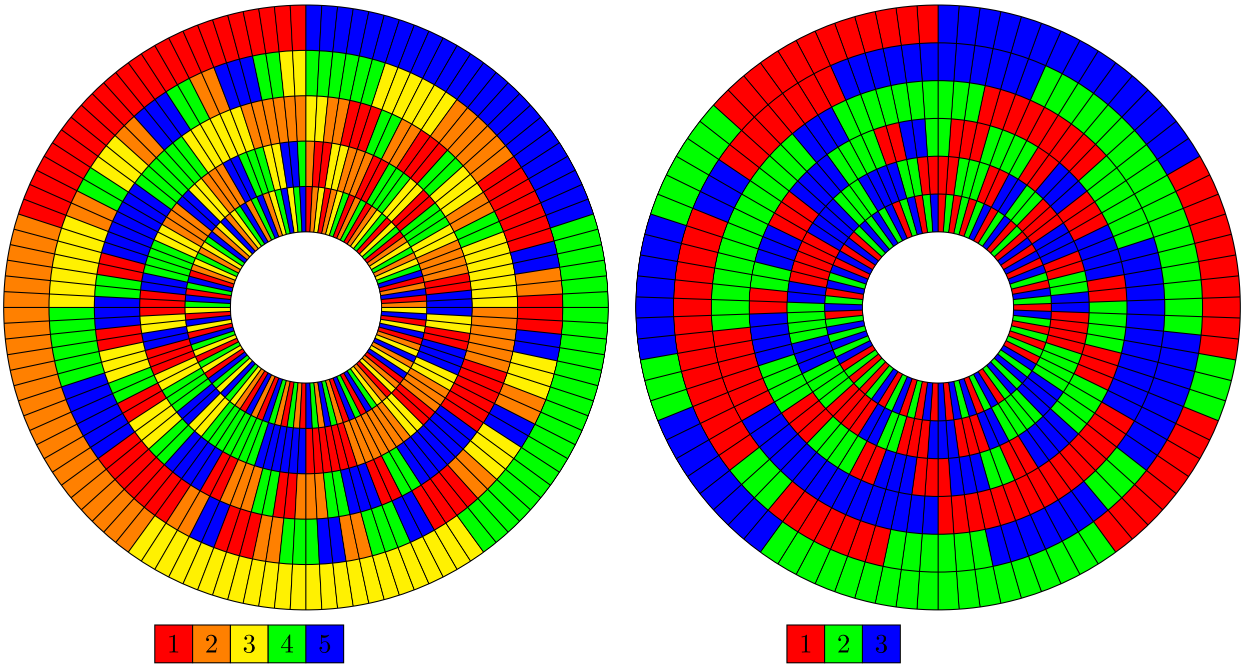


FIGURE 1. Star transposition Gray codes for $(4,4)$-combinations obtained from Theorem 1 for $n = 3$ and $s = 1, 2, \ldots, 6$. 1-bits are drawn as black squares, 0-bits as white squares. The initial block α_0 of the flip sequence is shown at the top, and the division of all $N = 70$ combinations into $2n + 1 = 7$ blocks of length $2C_n = 10$ is highlighted by horizontal lines.

1.5. **Related work.** Let us briefly discuss several results and open questions that are closely related to our work.

1.5.1. *Star transpositions for permutations.* In the literature, star transposition orderings of objects other than combinations have been studied intensively. A classical result, discovered independently by Kompel'maher and Liskovec [KL75] and Slater [Sla78], is that all *permutations* of $[n]$ can be generated (cyclically) by star transpositions, i.e., in every step, the first entry of the permutation is swapped with a later entry. An efficient algorithm for this task was



(a) $(a_1,\ldots,a_5)=(1,1,1,1,1)$ (b) $(a_1,a_2,a_3)=(2,2,2)$

Figure 2. Star transposition Gray codes for (a) permutations of length $n=5$ and (b) multiset permutations with frequencies $(a_1,a_2,a_3)=(2,2,2)$. Permutations are arranged in clockwise order, starting at 12 o'clock, with the first entry on the inner track, and the last entry on the outer track. The color on the inner track alternates in each step.

found by Ehrlich, and is described as Algorithm E in Knuth's book [Knu11, Section 7.2.1.2] (see also [SW13]). For instance, for $n=4$ such an ordering is given by starting at the identity permutation 1234 and applying the flip sequence $\alpha=12121321212312121321212 3$ (indices are again 0-based). The ordering of permutations resulting from this algorithm for $n=5$ is shown in Figure 2 (a). The first two of the aforementioned papers prove more generally that permutations can be generated using any set of transpositions that forms a connected graph as a basis, such as star transpositions or adjacent transpositions. Tchuente [Tch82] proved more generally that the graph of permutations under such transpositions is Hamilton-laceable for $n\geq 4$, i.e., it has a Hamilton path between any two permutations with opposite signs. These results are special cases of a more general open problem that asks whether the Cayley graph of the symmetric group on any set of generators has a Hamilton cycle, which in turn is a special case of an even more general conjecture attributed to Lovász about Hamilton cycles on arbitrary connected Cayley graphs [Lov70]; see [RS93, KM09, PR09] for more references in this direction.

1.5.2. *Multiset permutations.* Combinations and permutations are both special cases of *multiset permutations*. A multiset permutation is a string over the alphabet $\{1,\ldots,n\}$ with a given frequency distribution $(a_1,\ldots,a_n)$, i.e., the symbol i appears exactly a_i times in the string for all $i=1,\ldots,n$. For instance, 4412113 is a multiset permutation for $n=4$ with frequencies $(a_1,a_2,a_3,a_4)=(3,1,1,2)$. Clearly, for $n=2$ multiset permutations contain only two symbols, so they encode combinations. On the other hand, for $(a_1,\ldots,a_n)=(1,\ldots,1)$ every symbol appears exactly once, so such multiset permutations are simply permutations of $[n]$. Shen and Williams [SW19] raised a beautiful and brave conjecture which asserts that for any integers $n\geq 2$

and $k \geq 1$, all multiset permutations over the alphabet $\{1, \ldots, n\}$ with frequencies $(a_1, \ldots, a_n) = (k, \ldots, k)$ can be generated by star transpositions. The only confirmed general cases for this conjecture are the case $n = 2$ (the middle levels conjecture) and the case $k = 1$ (by the results on permutations mentioned before). In addition, Shen and Williams gave a solution for $(n, k) = (3, 2)$ in their paper, which is shown in Figure 2 (b). We also verified the next two small cases $(n, k) = (3, 3)$ and $(n, k) = (4, 2)$ by computer. Moreover, the techniques developed in this paper allowed us to solve Shen and Williams' conjecture for the cases $k \in \{2, 3, 4\}$ and $n \geq 2$ [FGMM20].

1.5.3. *Other algorithms for combination generation.* We also know many efficient algorithms for generating combinations that do not use star transpositions. Tang and Liu [TL73] first showed that all (k, ℓ)-combinations can be generated by transpositions of a 0-bit with a 1-bit, where neither of the swapped bits is required to be at the boundary. Their construction arises from restricting the classical binary reflected Gray code to bitstrings with k 1s, and was turned into a constant-time algorithm by Bitner, Ehrlich, and Reingold [BER76]. Eades and McKay [EM84] showed that (k, ℓ)-combinations can be generated by transpositions of the form $00 \ldots 01 \leftrightarrow 10 \ldots 00$, i.e., the bits between the swapped 0 and 1 are all 0s. We can think of this as an algorithm that plays all possible combinations of k keys out of $n = k + \ell$ available keys on a piano, without ever crossing any fingers. Jenkyns and McCarthy [JM95] showed that we can restrict the allowed swaps further and only allow transpositions of the form $01 \leftrightarrow 10$ or $001 \leftrightarrow 100$; see also [Cha89]. Eades, Hickey and Read [EHR84] and independently Buck and Wiedemann [BW84] proved that all (k, ℓ)-combinations can be generated by using only adjacent transpositions $01 \leftrightarrow 10$ if and only if $k \leq 1$ or $\ell \leq 1$ or $k \cdot \ell$ is odd. An efficient algorithm for this problem was given by Ruskey [Rus88].

Another elegant and efficient method for generating combinations based on prefix rotations was described by Ruskey and Williams [RW09]. An interesting open question in this context is whether all (k, ℓ)-combinations can be generated by prefix reversals, i.e., in each step, a prefix of the bitstring representation is reversed to obtain the next combination. Such orderings can be constructed easily for the cases $k \in \{1, 2\}$ or $\ell \in \{1, 2\}$, but no general construction is known.

1.6. **Proof ideas.** In this section we outline the main ideas used in our proof of Theorem 1, and in its algorithmization stated in Theorem 2. We also highlight the new contributions of our work compared to previous papers.

1.6.1. *Flipping through necklaces.* We start noting that the first bit of a star transposition ordering of combinations alternates in each step (see Figure 1), so we may simply omit it, and obtain an ordering of all bitstrings of length $2n + 1$ with either exactly n or $n + 1$ many 1s, such that in every step, a single bit is flipped. Observe that from a flip sequence α_0 that satisfies the conditions of Theorem 1 we can uniquely reconstruct the first bitstring of each block, by considering for each index $i \in \{1, \ldots, 2n + 1\}$ the parity of the position of first occurence of the number i in α starting from this block. For example, for the flip sequence α defined by $\alpha_0 := 6253462135$ and $s = 1$ (see the left column in Figure 1), the first occurence of the numbers $i = 1, \ldots, 7$ in α is at positions $7, 1, 3, 4, 2, 0, 10$ and the parity of those numbers is the starting bitstring 1110000. As any two consecutive blocks of the flip sequence differ by addition of s, the first bitstrings of the blocks differ by cyclic rotation by s positions. From this we obtain that the flip sequence α_0 that operates on these strings of length $2n + 1$ must visit every equivalence class of bitstrings under rotation exactly once, and it must return to a bitstring from the same equivalence class as the starting bitstring. It also follows that the compression factor $2n+1$ in Knuth's problem is best possible. Formally, a *necklace* $\langle x\rangle$ for a bitstring x is the set of all strings that are obtained as cyclic rotations of x. For example, the necklace of $x = 1110000$ is $\langle x\rangle = \{1110000, 1100001, 1000011, 0000111, 0001110, 0011100, 0111000\}$, and there are 10 necklaces for $n = 3$, namely $\langle 1110000\rangle$, $\langle 1101000\rangle$, $\langle 1100100\rangle$, $\langle 1100010\rangle$, $\langle 1010100\rangle$ and their complements. In the example shown in Figure 1, each of the flip sequences α_0 shown visits exactly one representative from each necklace, and it starts and ends with a bitstring from $\langle 1110000\rangle$. In fact, the order of necklaces is exactly the same for each of the columns in the figure, and the only difference are the chosen representatives. For example, in the first column ($s = 1$) we visit the bitstring 1010110 after three flips, and in the last column ($s = 6$) we visit the bitstring 1011010 after three flips, and both differ only by cyclic rotation. Moreover, all flip sequences in the figure start with the string 1110000 and end at a cyclic rotation of it after 10 flips, and the value s by which the string is rotated to the right after applying α_0 takes every possible value $s = 1,\ldots,6$. We refer to s as the *shift* of the flip sequence α_0. The crucial observation is that every string of length $2n+1$ with either exactly n or $n+1$ many 1s has exactly $2n+1$ distinct cyclic rotations, i.e., every necklace has the same size $2n+1$. Consequently, we may apply the shifted flip sequences α_i, obtained from α_0 by element-wise addition of $i\cdot s$ modulo $2n+1$, one after the other for $i = 1,\ldots,2n$, and this will produce the desired star transposition ordering of all $(n+1,n+1)$-combinations. Clearly, for this to work the shift s and $2n+1$ must be coprime, otherwise we will return to the starting bitstring prematurely before exhausting all bitstrings from the necklaces. In particular, if $s = 0$ we return to the starting bitstring after applying only α_0. For instance, applying the flip sequence $\alpha_0 = 6241247617$ to the starting string 1110000 visits every necklace exactly once, but returns to the exact same bitstring after 10 flips (every bit is flipped an even number of times by α_0), so this flip sequence has shift $s = 0$. This explains the condition stated in Theorem 1 that s and $2n+1$ must be coprime, which is necessary and cannot be omitted.

1.6.2. *Gluing flip sequences together.* To construct a flip sequence α_0 that visits every necklace exactly once and returns to the starting necklace, we first construct many disjoint shorter flip sequences that together visit every necklace exactly once. These basic flip sequences are obtained from a simple bitflip rule based on Dyck words that is invariant under cyclic rotations. In a second step, these basic flip sequences are glued together to a single flip sequence by local modifications.

Figure 3 illustrates this approach for $n = 3$. We may start at the bitstring $x_1 = 0010110$ and apply the flip sequence $\beta = 251642$ to generate a sequence of bitstrings $x_1, x_2, \ldots, x_6, x_1'$, and the final bitstring $x_1' = 1011000$ belongs to the same necklace as x_1, and it differs from x_1 by a right-rotation of $s_\beta = 5$. Similarly, from the bitstring $y_1 = 1101000$ we may apply the flip sequence $\gamma = 7152$ to generate a sequence of bitstrings y_1, y_2, y_3, y_4, y_1', and the final bitstring $y_1' = 0001101$ belongs to the same necklace as y_1, and it differs from y_1 by a right-rotation of $s_\gamma = 3$. The sets of necklaces

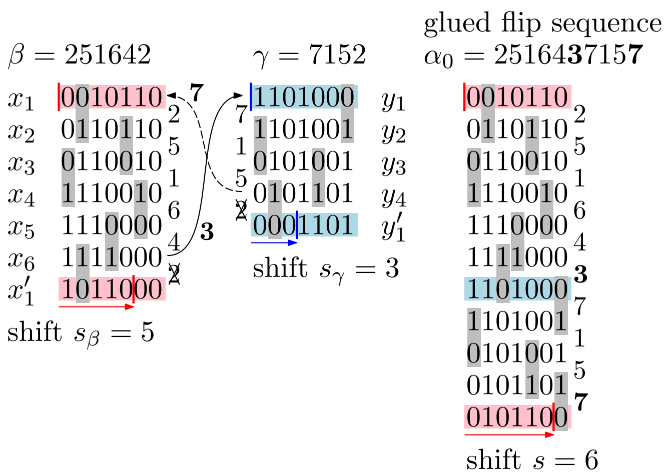


FIGURE 3. Gluing of flip sequences.

$\langle x_1\rangle,\ldots,\langle x_6\rangle$ and $\langle y_1\rangle,\ldots,\langle y_4\rangle$ visited by the two sequences are disjoint, and every necklace is contained in exactly one sequence. As x_6 differs from y_1 by a single flip of the 3rd bit, and y_4 differs from a cyclic rotation of x_1 by a single flip of the 7th bit, we may replace the last entry of β with 3 and the last entry of γ by 7, and concatenate the resulting sequences, yielding the flip sequence $\alpha_0 = 25164\mathbf{3}7157\mathbf{7}$, which visits every necklace exactly once. Moreover, the shift of the resulting flip sequence α_0 turns out to be $s = 6$ (which is coprime to $2n + 1 = 7$). In this example, the gluing of the two flip sequences is achieved by taking their symmetric difference with a 4-cycle of necklaces $(\langle x_1\rangle, \langle x_6\rangle, \langle y_1\rangle, \langle y_4\rangle)$, removing one flip from each of the two original sequences, and adding two flips to transition back and forth between them. In our proof later, for technical reasons the gluing of flip sequences uses slightly more complicated structures, namely 6-cycles of necklaces, albeit with the same effect of joining two smaller flip sequences to one in each step. One of the major technical hurdles is to ensure that several of these gluing steps do not interfere with each other.

The benefit of the gluing approach is that Knuth's generation problem translates into the problem of finding a spanning tree in a suitably defined auxiliary graph: Specifically, the nodes of this auxiliary graph are the basic flip sequences we start with, and the edges correspond to the gluing 6-cycles that join two of them together. A spanning tree in the auxiliary graph corresponds to a collection of gluing 6-cycles that glue together all basic flip sequences to a single flip sequence α_0 with the desired properties. We show that each of our basic flip sequences can be interpreted combinatorially as a plane tree with n edges (in particular, the number of basic flip sequences is given by the number of these trees), so the aforementioned auxiliary graph has all plane trees with n edges as its nodes; see Figure 4. Moreover, the gluing operation between two basic flip sequences can be interpreted as a local modification of the two plane trees involved. Specifically, a leaf of one plane tree is removed and reattached to a neighbor of the original attachment vertex. A spanning tree in the auxiliary graph can be obtained by choosing a minimal set of gluing 6-cycles such that the corresponding local modifications allow to transform any two plane trees into each other (see the bold edges in Figure 4).

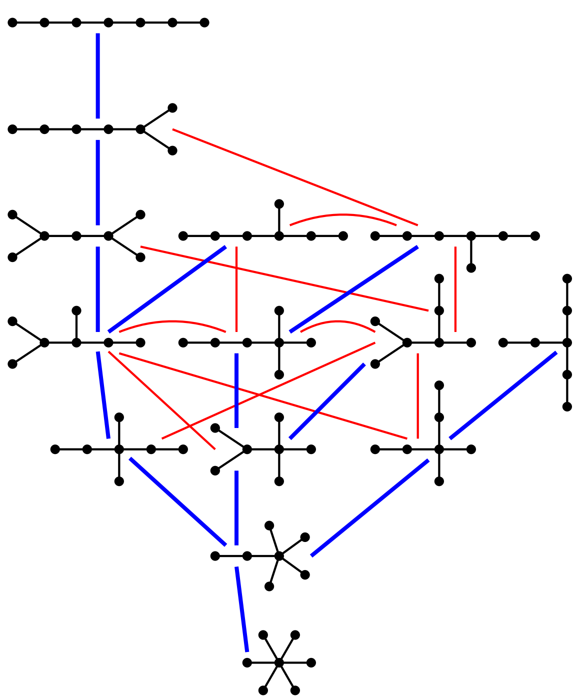


FIGURE 4. Auxiliary graph on plane trees with $n = 6$ edges. Edges correspond to local modification operations on the plane trees. The bold edges show a spanning tree in the graph.

1.6.3. *Controlling the shift.* The next key step is to control the shift of the resulting flip sequence α_0. Without controlling the overall shift, we may end up with a shift $s = 0$, which is useless as explained above, or more generally, with a shift s that is not coprime to $2n+1$, which is again useless. Even if we managed to obtain a shift s that is coprime to $2n+1$, Knuth's problem specifically asks for a shift of $s = 1$, which is the most natural choice to state the problem. Consequently, we need to be able to change the shift from any number s to 1 modulo $2n + 1$.

However, if we can do that, then we can also change the shift from any number s to any other number that is coprime to $2n+1$, as we made no assumptions on which s we get initially. In this sense, being able to solve Knuth's problem, which asks for a shift of 1, is not easier than solving the general problem stated in Theorem 1, which allows for arbitrary shifts (coprime to $2n+1$).

Ideally, gluing two flip sequences with shifts s_β and s_γ should give a flip sequence with shift $s_\beta + s_\gamma$. This would allow us to compute the overall shift simply as the sum of shifts of the basic flip sequences, and this sum can be evaluated explicitly to be $s = C_n$, the nth Catalan number. In the example from the previous section, we had $s_\beta = 5$ and $s_\gamma = 3$, and an overall shift of $s = 6$ after the gluing, which is different from $s_\beta + s_\gamma = 5 + 3 = 8 = 1$ (modulo 7), so the desired additivity of shifts under gluing does not hold in this example. In fact, guaranteeing that the shifts behave additively under gluing requires substantial effort, and is achieved by constructing a particularly nice spanning tree in the aforementioned auxiliary graph.

Having guaranteed that the overall shift is $s = C_n$, we apply two complementary techniques for modifying the shift to any desired value (coprime to $2n+1$) that we discuss in the following.

The first approach to modify the shift of flip sequences we refer to as *switching*. To illustrate this technique, consider again the columns $s = 1$ and $s = 6$ in Figure 1. As we mentioned before, both flip sequences visit the same necklaces in the same order, but they only differ in the chosen necklace representatives, yielding different shift values. Specifically, after the first two flips, both flip sequences α_0 for $s = 1$ and $s = 6$ visit the bitstring $x = 1010010$; see Figure 5. In the third step, one sequence flips the 5th bit of x, yielding the string $y = 1010110$, while the other sequence flips the 4th bit of x, yielding the string $y' = 1011010$, which only differ by cyclic right-rotation by 5 steps. After this flip, the entries of both flip sequences differ only by the constant 5, and consequently, their shift values differ only by 5 ($s = 1$ and $s = 6$). We refer to a bitstring x that allows flipping two distinct bits to reach two bitstrings y and y' in the same necklace $\langle y \rangle = \langle y' \rangle$ as a *switch*. We systematically construct many possible switches that allow modifying the shift of flip sequences in a controlled way, while preserving the order of the visited necklaces. Unfortunately, we are unable to prove that the basic flip sequences we use always contain enough of those switches that are usable for us, even though computer experiments suggest that this is the case. This is why we use the switching method only to prove Theorem 1 for small values of $n \leq 38$ (these are probably all values that are ever interesting in 'practice').

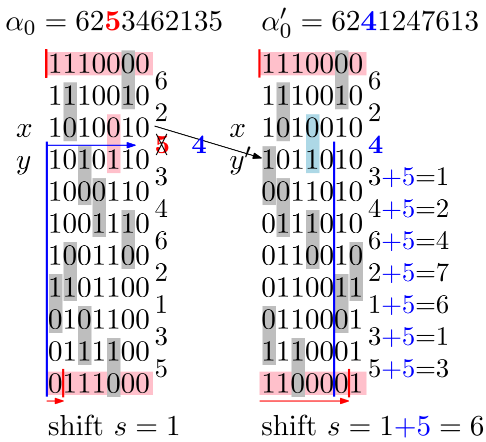


FIGURE 5. Controlling the shift value of flip sequences by switching.

For $n \geq 39$ we employ another method to modify the shift of flip sequences, which works by modifying the aforementioned spanning tree in the auxiliary graph. This method changes the order in which necklaces are visited, unlike the switching method discussed before, which affects only the chosen representatives. Also, the spanning tree modification does not work for $n \leq 38$, as there are not enough plane trees available, which form the nodes of the auxiliary graph (recall Figure 4).

1.6.4. *Efficient algorithms.* The biggest obstacle in translating our constructive proof into an efficient algorithm is to quickly compute the resulting shift s of the flip sequence α_0 that results from the gluing process. Only with this information we know by how much s needs to be modified to achieve the shift value that is specified in the input of the algorithm (which may be different from s). For this we crucially need the addivitity of the shift values under gluing, which guarantees that $s = C_n$. Clearly, the nth Catalan number modulo $2n+1$ can be computed efficiently. For instance, for $n = 10$ we have $s = C_n = 16796 = 17 \pmod{2n+1}$, and if the desired shift value is 1, we know that we need to correct s by -16 in the course of the algorithm. Similar to our proof of Theorem 1, our algorithm also distinguishes between two regimes, one for small $n \leq 38$, where those modifications are done via switching, and one for $n \geq 39$, where the corrections are based on spanning tree modifications.

1.6.5. *Comparison to previous work.* The general idea of gluing, and the resulting reduction to a spanning tree problem, is very natural and variations of it have been used successfully in several papers before (see e.g. [CW93, HRW12, Hol17, SW18, MNW18, GMM20]). As mentioned before, a flip sequence α_0 satisfying the requirements of Knuth's conjecture encodes the entire flip sequence α by a factor of $2n+1$ more compactly. This requires us to perform all the aforementioned steps, i.e., the construction of basic flip sequences and gluing them together, on *necklaces* rather than on *bitstrings*, as was previously done in [Müt16, GMN18], which creates many additional technical complications. The key innovation of our paper is to develop these necklace-based constructions, and in particular, to control the shift of the resulting flip sequence α_0, using the techniques presented in Section 1.6.3. The flexibility that these methods have will certainly yield other interesting applications in the future. As evidence for that, recall from Section 1.5.2 that these techniques allow us to construct solutions for Shen and Williams' conjecture on multiset permutations with frequencies $(a_1, \ldots, a_n) = (k, \ldots, k)$ for the cases $k \in \{2, 3, 4\}$ and $n \geq 2$ [FGMM20]. We are confident that with more work, they will enable us to settle also this problem in full generality.

1.7. **Outline of this paper.** In Section 2 we introduce some terminology and notation that is used throughout the paper. In Section 3 we explain the construction of the basic flip sequences that together traverse all necklaces. In Section 4 we discuss the gluing technique that we use to join the basic flip sequences together to a single flip sequence that satisfies the conditions of Theorem 1. These two ingredients are combined in Section 5, where we reduce Knuth's problem to a spanning tree problem in a suitably defined auxiliary graph, and we present the proof of Theorem 1 for $n \geq 39$ based on the aforementioned spanning tree modification technique. In Section 6 we redefine the spanning tree in the auxiliary graph, so that shift values behave additively under gluing, which is essential for our algorithms and also for our proof of Theorem 1 for small n. In Section 7 we discuss the switching technique, which is then used to prove Theorem 1 for $n \leq 38$. The proof of Theorem 2 is explained in Section 8.

2. Preliminaries

In this section we introduce some definitions and easy observations that we will use repeatedly in the subsequent sections.

2.1. **Binary strings and necklaces.** We let A_n and B_n denote all bitstrings of length $2n+1$ with exactly n or $n+1$ many 1s, respectively. The *middle levels graph* M_n has $A_n \cup B_n$ as its vertex set, and an edge between any two bitstrings that differ in a single bit. As mentioned in Section 1.6.1 before, in a star transposition ordering of all $(n+1, n+1)$-combinations, the first bit alternates between 0 and 1 in each step; see Figure 1. Consequently, omitting the first bit, we see a Hamilton cycle in the graph M_n on the remaining $2n+1$ bits. We index these bit

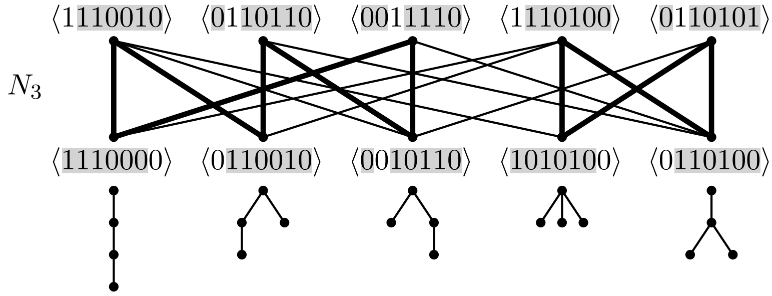


FIGURE 6. The necklace graph N_3, with the cycle factor $\mathcal{F}_3$ highlighted. The Dyck words in the necklace representatives are highlighted by gray boxes, and the corresponding rooted trees $t(x)$ for all $\langle x\rangle$, $x \in A_3$, are shown at the bottom.

positions by $1, \ldots, 2n+1$, and we consider all indices modulo $2n+1$ throughout this paper, with $1, \ldots, 2n+1$ as residue class respresentatives (rather than $0, \ldots, 2n$).

The empty bitstring is denoted by ε. For any bitstring x and any integer $i \geq 0$, we let x^i denote the bitstring obtained by concatenating i copies of x. Also, we let $\sigma^i(x)$ denote the bitstring obtained from x by cyclic left-rotation by i positions. As mentioned before, the *necklace of* x, denoted $\langle x\rangle$, is defined as the set of all bitstrings obtained from x by cyclic rotations, i.e., we have $\langle x\rangle = \{\sigma^i(x) \mid i \geq 0\}$. E.g., for $x = 11000 \in A_2$ we have $\langle x\rangle = \{11000, 10001, 00011, 00110, 01100\}$. The *necklace graph* N_n has as vertex set all $\langle x\rangle$, $x \in A_n \cup B_n$, and an edge between any two necklaces $\langle x\rangle$ and $\langle y\rangle$ for which x and y differ in a single bit; see Figure 6. Observe that N_n arises as the quotient of M_n under the equivalence relation of rotating bitstrings cyclically. Note that for a given necklace $\langle x\rangle$, there may be two distinct bits in the representative x that reach the same necklace $\langle y\rangle$, a fact that we will exploit heavily in Section 7. Nonetheless, we still consider N_n as a simple graph, and so not all vertices of N_n have the same degree. As mentioned before, for any $x \in A_n \cup B_n$, the necklace $\langle x\rangle$ has size $2n+1$, i.e., the graph N_n has by a factor $2n+1$ fewer vertices than the graph M_n. To define the flip sequence α_0 in Theorem 1, we will construct a Hamilton cycle in N_n. This is achieved using paths in the middle levels graph M_n that have the following property: A path $P = (x_1, \ldots, x_k)$ in M_n is called *periodic*, if one can flip a single bit in x_k to obtain a vertex x_{k+1} that satisfies $\langle x_{k+1}\rangle = \langle x_1\rangle$.

2.2. **Operations on sequences.** For any sequence $x = (x_1, \ldots, x_k)$, we let $|x| := k$ denote the length of the sequence. For any sequence of integers $x = (x_1, \ldots, x_k)$ and any integer a, we define $x + a := (x_1 + a, \ldots, x_k + a)$. For any sequence of bitstrings $x = (x_1, \ldots, x_k)$, we define $\langle x\rangle := (\langle x_1\rangle, \ldots, \langle x_k\rangle)$ and $\sigma^i(x) := (\sigma^i(x_1), \ldots, \sigma^i(x_k))$.

2.3. **Dyck words, rooted trees, and plane trees.** The *excess* of a bitstring x is the number of 1s minus the number of 0s in x. If x has excess 0 (i.e., it has the same number of 1s and 0s) and every prefix of x has non-negative excess, then we call x a *Dyck word*. We use D_n to denote the set of all Dyck words of length $2n$. Moreover, we define $D := \bigcup_{n\geq 0} D_n$.

An (ordered) *rooted tree* is a rooted tree with a specified left-to-right ordering for the children of each vertex. Every Dyck word $x \in D_n$ can be interpreted as a rooted tree with n edges as follows; see Figure 7: If $x = \varepsilon$, then this corresponds to the tree that has an isolated vertex as root. If $x \neq \varepsilon$, then it can be written uniquely as $x = 1\,u\,0\,v$ with $u, v \in D$. We then consider the trees L and R corresponding to u and v, respectively, and the tree corresponding to x has L rooted at the leftmost child of the root, and the edges from the root to all other children except the leftmost one, together with their subtrees, form the tree R.

Given a rooted tree x, let $\rho(x)$ denote the tree obtained by rotating the tree to the right, which corresponds to designating the leftmost child of the root of x as the new root in $\rho(x)$. In terms of bitstrings, if $x = 1\,u\,0\,v$ with $u, v \in D$, then $\rho(x) = u\,1\,v\,0$; see Figure 7.

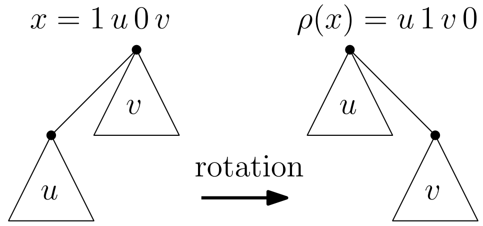


FIGURE 7. Interpretation of Dyck words as rooted trees and definition of tree rotation.

A *plane tree* is a tree with a specified cyclic ordering of the neighbors of each vertex. We think of it as a tree embedded in the plane, where the cyclic ordering is the ordering of the neighbors of each vertex in counterclockwise (ccw) direction around the vertex. We let T_n denote the set of all plane trees with n edges. For any rooted tree x, we let $[x]$ denote the set of all rooted trees obtained from x by rotation, i.e., we define $[x] := \{\rho^i(x) \mid i \geq 0\}$, and this can be interpreted as the plane tree underlying x, obtained by 'forgetting' the root. We also define $\lambda(x) := |[x]|$, and for the plane tree $T = [x]$ we define $\lambda(T) := \lambda(x)$. Note that $\lambda(x) = \min\{i \geq 1 \mid \rho^i(x) = x\}$.

For any plane tree T and any of its edges (a, b), we let $T^{(a,b)}$ denote the rooted tree obtained from T by designating a as root such that b is its leftmost child. Moreover, we let $T^{(a,b)-}$ denote the rooted tree obtained from $T^{(a,b)}$ by removing all children and their subtrees of the root except the leftmost one, and we let $T^{(a,b)--}$ denote the tree obtained as the subtree of $T^{(a,b)-}$ that is rooted at the vertex b. Given a vertex a of T, consider each neighbor b_i, $i = 1, \ldots, k$, of a and define the rooted tree $t_i := T^{(a,b_i)-}$. We refer to the rooted trees $t_1, \ldots, t_k$ as the *a-subtrees* of T. Note that we have $T = [(t_1, \ldots, t_k)]$.

A *leaf* of a rooted or plane tree is a vertex with degree 1. In particular, the root of a rooted tree is a leaf, if and only if it has exactly one child. We say that a leaf of a tree is *thin*, if its unique neighbor in the tree has degree at most 2, otherwise we call the leaf *thick*. For any rooted or plane tree T, we write $v(T)$ and $e(T)$ for the number of vertices or edges of T, respectively.

2.4. **Centroids and potential.** Given a (rooted or plane) tree T, the *potential of a vertex a*, denoted $\varphi(a)$, is the sum of distances from a to all other vertices in T. The *potential of the tree T*, denoted $\varphi(T)$, is the minimum of $\varphi(a)$ over all vertices a of T. A *centroid* of T is a vertex a with $\varphi(a) = \varphi(T)$.

Our first lemma captures important properties of a centroid of a tree.

Lemma 3. *Let T be a plane tree. For every edge (a, b) of T, we have*

$$\varphi(b) - \varphi(a) = e(T^{(b,a)--}) - e(T^{(a,b)--}). \tag{1}$$

As a consequence, T has either one centroid or two adjacent centroids. If $e(T)$ is even, then T has exactly one centroid.

Proof. Comparing the potentials of b and a, note that the distance of every vertex in $T^{(b,a)--}$ to b differs by $+1$ from its distance to a. Conversely, the distance of every vertex in $T^{(a,b)--}$ to b differs by -1 from its distance to a. Combining these observations shows that $\varphi(b) = \varphi(a) + v(T^{(b,a)--}) - v(T^{(a,b)--})$. Using that $v(T) = e(T) + 1$ for both trees $T \in \{T^{(b,a)--}, T^{(a,b)--}\}$, we obtain (1). Consider any path between two leaves of T. By (1), the sequence of potential differences along this path forms a strictly decreasing sequence. It follows that T has either one or two centroids, and if there are two, then they must be adjacent in T. Moreover, if there are two centroids a and b, then we must have $\varphi(b)-\varphi(a)=0$ along the edge (a,b) of T, and then (1) implies that $e(T^{(b,a)--})=e(T^{(a,b)--})$, i.e., $e(T)=e(T^{(b,a)--})+e(T^{(a,b)--})+1=2e(T^{(a,b)--})+1$ is odd. □

The next lemma describes possible values that the parameter $\lambda(T)$ can take for a plane tree T.

Lemma 4. *Let $T\in T_n$ be a plane tree with $n\geq 1$ edges. Then $\lambda(T)$ is a divisor of $2n$. If T has a unique centroid, then $\lambda(T)$ is even, and if T has two centroids, then $\lambda(T)=2n$ if n is even, and $\lambda(T)\in\{n,2n\}$ if n is odd. Moreover, for $n\geq 4$ and any even divisor k of $2n$ or for $k=n$ there is a plane tree T with $\lambda(T)=k$.*

Proof. Let x be a rooted tree such that $T=[x]$. Note that $x=T^{(a,b)}$ for some edge (a,b) of T. As there are at most $2n$ choices for the pair (a,b), we obtain that $\lambda(T)\leq 2n$. If $\lambda:=\lambda(T)<2n$, then we clearly have $\rho^{\lambda}(x)=x$ and $\rho^{2n}(x)=x$. If λ was not a divisor of $2n$, then there are integers $c\geq 1$ and $1\leq d<\lambda$ such that $2n=c\lambda+d$, and together the previous two equations would yield $\rho^{d}(x)=x$, and then $d<\lambda$ would contradict the definition of λ. We conclude that $\lambda(T)$ is indeed a divisor of $2n$.

Now suppose that T has a unique centroid c. Consider the c-subtrees $t_1,\ldots,t_k$ of T, i.e., we have $T=[(t_1,\ldots,t_k)]$. Each t_i, $i=1,\ldots,k$, contributes either 0 or $2e(t_i)$ to the quantity $\lambda(T)$. This shows that $\lambda(T)$ is even.

It remains to consider the case that T has two centroids c and c'. We define the rooted trees $t_c:=T^{(c',c)--}$ and $t_{c'}:=T^{(c,c')--}$. If n is even, then $n-1$ is odd, implying that $e(t_c)\neq e(t_{c'})$. This yields in particular that $t_c\neq t_{c'}$, and so we have

$$\lambda(T)=2e(t_c)+2e(t_{c'})+2=2\underbrace{\left(e(t_c)+e(t_{c'})+1\right)}_{=n}=2n. \tag{2}$$

The $+2$ in (2) comes from the two rooted trees $T^{(c,c')}$ and $T^{(c',c)}$. If n is odd, then if $t_c\neq t_{c'}$ we also have (2), i.e., $\lambda(T)=2n$, whereas if $t_c=t_{c'}$, then we have

$$\lambda(T)=2e(t_c)+1=e(t_c)+e(t_{c'})+1=n. \tag{3}$$

The $+1$ in (3) comes from the rooted tree $T^{(c,c')}=T^{(c',c)}$.

To prove the last part of the lemma, let $k<n$ be an even divisor of $2n$, i.e., we have $2n=kd$ for some integer $d\geq 3$ and $k=2\ell$ for some integer $\ell\geq 1$. Consider the plane tree T obtained by gluing together d copies of the path on ℓ edges at a common centroid vertex. This tree has $d\ell=dk/2=n$ edges and satisfies $\lambda(T)=2\ell=k$. For $k=n$, the path T on n edges satisfies $\lambda(T)=n$. For $k=2n$, the path T on $n-1$ edges, with an extra edge appended to one of its interior vertices, satisfies $\lambda(T)=2n$ under the assumption that $n\geq 4$. □

3. Periodic paths

In this section we define the basic flip sequences that together visit every necklace exactly once, following the ideas outlined in Sections 1.6.1 and 1.6.2. We thus obtain a so-called *cycle factor* in the necklace graph N_n, i.e., a collection of disjoint cycles that visit every vertex of the graph exactly once. The key properties of these cycles that we will need later are summarized in Proposition 7 below. Each cycle in the necklace graph N_n is obtained from a periodic path in the middle levels graph M_n, and we define these periodic paths via a simple bitflip rule based on Dyck words.

The following lemma is well-known (see [Bol06, Problem 7]).

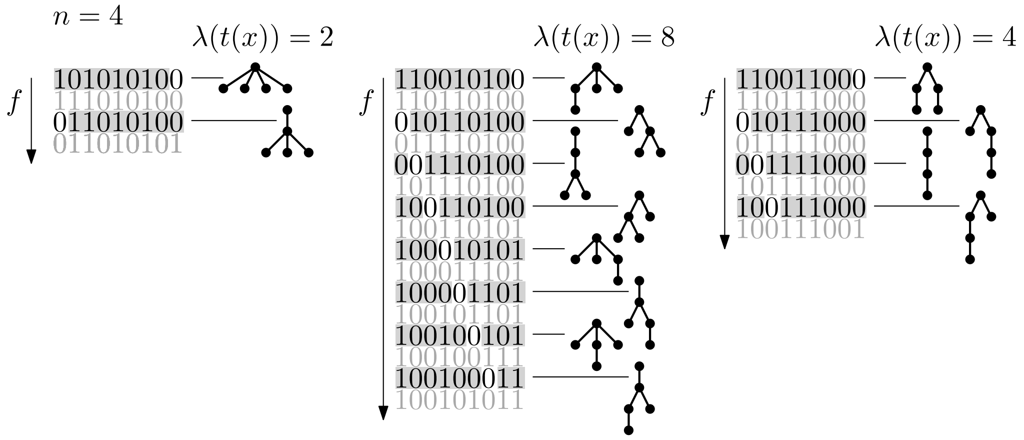


FIGURE 8. Definition of the function f for $n = 4$. The Dyck words in the bitstrings are highlighted by gray boxes, and the corresponding rooted trees $t(x)$ for the shown bitstrings $x \in A_4$, are displayed at the side. Bitstrings from the set B_4 are shown in gray. Consecutive trees in each column differ by tree rotation. As rotating the last tree yields the first tree in each column, the cycles in the necklace graph defined by f wrap around at the bottom and top.

Lemma 5. *For any $x \in A_n$, there is a unique integer $\ell = \ell(x)$ with $0 \le \ell \le 2n$ such that the first $2n$ bits of $\sigma^\ell(x)$ are a Dyck word. For any $y \in B_n$, there is a unique integer $\ell = \ell(y)$ with $0 \le \ell \le 2n$ such that the last $2n$ bits of $\sigma^\ell(y)$ are a Dyck word.*

For any $x \in A_n$, we let $t(x) \in D_n$ denote the first $2n$ bits of $\sigma^\ell(x)$ where $\ell := \ell(x)$, i.e., we have $\sigma^\ell(x) = t(x)\,0$. Similarly, for any $y \in B_n$, we let $t(y) \in D_n$ denote the last $2n$ bits of $\sigma^\ell(y)$ where $\ell := \ell(y)$, i.e., we have $\sigma^\ell(y) = 1\,t(y)$. In the following it will be crucial to consider the rooted trees corresponding to $t(x)$ and $t(y)$. By Lemma 5, every bitstring $x \in A_n \cup B_n$ can be identified uniquely with the rooted tree $t(x)$ and the integer $\ell(x)$.

Consider an $x \in A_n$ with $\ell(x) = 0$, i.e., we have

$$x = \underbrace{1\,u\,0\,v}_{t(x)}\,0 \tag{4a}$$

with $u, v \in D$. Then we define

$$y := f(x) = 1\,\underbrace{u\,1\,v\,0}_{\rho(t(x))} \in B_n. \tag{4b}$$

Note that we have $\ell(y) = 0$. We then define

$$f(y) = f(f(x)) := 0\,\underbrace{u\,1\,v\,0}_{\rho(t(x))} \in A_n. \tag{4c}$$

Note that we have $\ell(f(y)) = 1$. We extend these definitions to all $x \in A_n \cup B_n$ by setting

$$f(x) := \sigma^{-\ell}(f(\sigma^\ell(x))), \text{ where } \ell := \ell(x). \tag{4d}$$

This definition is illustrated in Figure 8. It follows directly from these definitions that the mapping $f : A_n \cup B_n \to A_n \cup B_n$ is invertible.

From (4) we obtain that for all $x \in A_n$ we have

$$t(f(f(x))) = t(f(x)) = \rho(t(x)). \tag{5}$$

Moreover, (4a)–(4c) show that if $\ell(x) = 0$, then we have $\ell(f(x)) = 0$ and $\ell(f(f(x))) = 1$. From this and (4d), we thus obtain for all $x \in A_n$ that

$$\ell(f(x)) = \ell(x) \quad \text{and} \quad \ell(f(f(x))) = \ell(x) + 1. \tag{6}$$

In words, if we cyclically read a bitstring $x \in A_n$ starting at position $p := \ell(x)+1$ and consider the first $2n$ bits as a rooted tree, ignoring the extra 0-bit, then the bitstring $f(x)$ read starting from position p has the extra 1-bit plus the rotated tree, and the bitstring $f(f(x))$ read starting from position $p+1$ is the same rotated tree plus the extra 0-bit.

For any $x \in A_n \cup B_n$, we define the integer

$$k(x) := \min\{i > 0 \mid \langle f^i(x)\rangle = \langle x\rangle\}. \tag{7}$$

The following lemma summarizes important properties of the parameter $k(x)$.

Lemma 6. *For every $x \in A_n \cup B_n$ we have the following:*

(i) For any $y \in \langle x\rangle$ and any integer $i \geq 0$ we have $\langle f^i(x)\rangle = \langle f^i(y)\rangle$. In particular, we have $k(y) = k(x)$.
(ii) For any integer $i \geq 0$ we have $\langle f^i(x)\rangle = \langle f^{k(x)+i}(x)\rangle$.
(iii) For any integers $0 \leq i < j < k(x)$ we have $\langle f^i(x)\rangle \neq \langle f^j(x)\rangle$.
(iv) For any integer $i \geq 0$ we have $k(f^i(x)) = k(x)$.
(v) We have $k(x) = 2\lambda(t(x))$.

Proof. (i) This follows directly from (4d).

(ii) By the definition of $k(x)$, we have $\langle x\rangle = \langle f^{k(x)}(x)\rangle$. Using (4d), this gives $\langle f^i(x)\rangle = \langle f^i(f^{k(x)}(x))\rangle = \langle f^{k(x)+i}(x)\rangle$.

(iii) Suppose for the sake of contradiction that $y := f^i(x)$ and $z = f^j(x)$ with $0 \leq i < j < k(x)$ satisfy $\langle y\rangle = \langle z\rangle$. Then, using that f is invertible, we obtain from (4d) that $\langle x\rangle = \langle f^{-i}(y)\rangle = \langle f^{j-i}(z)\rangle$ with $j - i < k(x)$, contradicting the definition of $k(x)$ in (7).

(iv) It suffices to prove that $k(f(x)) = k(x)$. Observe that we have $\langle f^{k(x)}(f(x))\rangle = \langle f^{k(x)+1}(x)\rangle = \langle f(x)\rangle$ by (ii). On the other hand, we have $\langle f^j(f(x))\rangle \neq \langle f(x)\rangle$ for all $1 \leq j < k(x)$ by (iii). Combining these two observations proves that $k(f(x)) = k(x)$.

(v) By (5), two applications of f correspond to one rotation of the tree $t(x)$. The statement now follows from the definition (7). □

For any $x \in A_n \cup B_n$ we define

$$P(x) := (x, f(x), f^2(x), \ldots, f^{k(x)-1}(x)). \tag{8a}$$

By (7), $P(x)$ is a periodic path in the middle levels graph M_n, and by Lemma 6 (iii), $\langle P(x)\rangle$ is a cycle in the necklace graph N_n. For any $y \in \langle x\rangle$ and any integer $i \geq 0$, combining Lemma 6 (i)+(iv) shows that $k(f^i(y)) = k(x)$, and so $\langle P(x)\rangle$ and $\langle P(f^i(y))\rangle$ describe the same cycle, differing only in the choice of the starting vertex (recall (4d)). We may thus define a cycle factor in N_n by

$$\mathcal{F}_n := \{\langle P(x)\rangle \mid x \in A_n \cup B_n\}. \tag{8b}$$

This definition is illustrated in Figures 6 and 8 for $n = 3$ and $n = 4$, respectively. The following proposition summarizes the observations from this section.

Proposition 7. *For any $n \geq 2$, the cycle factor $\mathcal{F}_n$ defined in* (8) *has the following properties:*

(i) For every $x \in A_n \cup B_n$, the $2i$th vertex y after x on the periodic path $P(x)$ satisfies $t(y) = \rho^i(t(x))$. Consequently, we can identify the path $P(x)$ and the cycle $\langle P(x)\rangle$ with the plane tree $[t(x)]$.

(ii) The number of vertices of the path $P(x)$ and the cycle $\langle P(x)\rangle$ is $2\lambda(t(x)) \geq 4$, and we have $\ell(f^{2i}(x)) = \ell(x) + i$ for all $i = 0, \ldots, \lambda(t(x))$.
(iii) The cycles of $\mathcal{F}_n$ are in bijection with plane trees with n edges.

Proof. Clearly, (i) follows from (5) and the definition (8a). Moreover, (iii) is an immediate consequence of (i). To prove (ii), note that $|P(x)| = k(x)$ by the definition (8a), and use that $k(x) = 2\lambda(t(x))$ by Lemma 6 (v). As $n \geq 2$, Lemma 4 guarantees that $\lambda(t(x)) \geq 2$, and so $|P(x)| = 2\lambda(t(x)) \geq 4$. The second part of claim (ii) follows directly from (6). □

4. Gluing the periodic paths

In this section we implement the ideas outlined in Section 1.6.2, showing how to glue pairs of periodic paths to one longer periodic path. It turns out that the gluing operation involving two periodic paths can be interpreted as a local modification operation on the two corresponding rooted trees; see Figure 9. Repeating this gluing process will eventually produce a single periodic path that corresponds to a Hamilton cycle in the necklace graph. The most technical aspect of this approach is to ensure that multiple gluing steps do not interfere with each other, and the conditions that ensure this are captured in Proposition 10 below.

We define the two rooted trees $s_n := 1(10)^{n-1}0 \in D_n$ for $n \geq 3$ and $s'_n := 10s_{n-1} \in D_n$ for $n \geq 4$. Note that both s_n and s'_n have n edges, s_n is a star, and s'_n is obtained from a star by appending an additional edge to one leaf. For $n \geq 4$, consider two Dyck words $x, y \in D_n$, $n \geq 4$, with $(x, y) \neq (s_n, s'_n)$ of the form

$$x = 1\,1\,0\,u\,0\,v, \quad y = 1\,0\,1\,u\,0\,v, \quad \text{with } u, v \in D. \tag{9}$$

We refer to (x, y) as a *gluing pair*, and we use G_n to denote the set of all gluing pairs (x, y), $x, y \in D_n$. Considering the corresponding rooted trees, we say that y is obtained from x by the *pull* operation, and we refer to the inverse operation that transforms y into x as the *push* operation; see Figure 9. We write this as $y = \text{pull}(x)$ and $x = \text{push}(y)$. We refer to any x as in (9) as a *pullable tree*, and to any y as in (9) as a *pushable tree*. Also, we refer to the subtrees u and v in (9) as the *left and right subtree of x or y*, respectively. A pull removes the leftmost edge that leads from the leftmost child of the root of x to a leaf, and reattaches this edge as the leftmost child of the root, yielding the tree $y = \text{pull}(x)$. A push removes the leaf that is the leftmost child of the root of y, and reattaches this edge as the leftmost child of the second child of the root of y, yielding the tree $x = \text{push}(y)$. Under this viewpoint, we can use the same identifiers for vertices and edges in x and y.

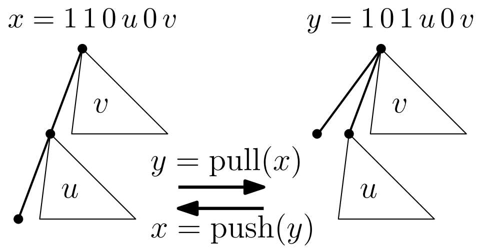


Figure 9. A gluing pair (x, y) and the pull/push operations between the corresponding rooted trees.

The next lemma asserts that the centroid(s) of a tree are invariant under certain pull/push operations, and that these operations change the tree potential only by ± 1.

Lemma 8. *Let $(x, y) \in G_n$ be a gluing pair as in (9). Every centroid of x contained in its right subtree is also a centroid of y, and we have $\varphi(y) = \varphi(x) - 1$. Every centroid of y contained in its left subtree is also a centroid of x, and we have $\varphi(x) = \varphi(x) + 1$.*

Proof. Let a be the leaf incident to the edge in which x and y differ. Clearly, a is not a centroid of y. Moreover, for any vertex b in the subtree u of x, the pull operation that transforms x

into y changes the potential of b by $+1$. Similarly, for any vertex b in the subtree v of x, the pull operation changes the potential of b by -1. This proves the first part of the lemma. The proof of the second part is analogous. □

For a gluing pair $(x,y) \in G_n$, we define $x^k := f^k(x\,0)$ and $y^k := f^k(y\,0)$ for $k \geq 0$. These sequences agree with the first vertices of the periodic paths $P(x)$ and $P(y)$, respectively, defined in (8a). Using the definition (4), a straightforward calculation yields

$$\begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \\ x^4 \\ x^5 \\ x^6 \end{pmatrix} = \begin{pmatrix} 1\,1\,0\,u\,0\,v\,0 \\ 1\,1\,0\,u\,1\,v\,0 \\ 0\,1\,0\,u\,1\,v\,0 \\ 0\,1\,1\,u\,1\,v\,0 \\ 0\,0\,1\,u\,1\,v\,0 \\ 1\,0\,1\,u\,1\,v\,0 \\ 1\,0\,0\,u\,1\,v\,0 \end{pmatrix}, \quad \begin{pmatrix} y^0 \\ y^1 \end{pmatrix} = \begin{pmatrix} 1\,0\,1\,u\,0\,v\,0 \\ 1\,1\,1\,u\,0\,v\,0 \end{pmatrix}. \tag{10}$$

From this we obtain

$$\begin{pmatrix} t(x^0) \\ t(x^2) = \rho(t(x^0)) \\ t(x^4) = \rho^2(t(x^0)) \\ t(x^6) = \rho^3(t(x^0)) \end{pmatrix} = \begin{pmatrix} 1\,1\,0\,u\,0\,v \\ 1\,0\,u\,1\,v\,0 \\ 1\,u\,1\,v\,0\,0 \\ u\,1\,v\,0\,1\,0 \end{pmatrix}, \quad t(y^0) = (1\,0\,1\,u\,0\,v\,0) \tag{11}$$

(recall Proposition 7 (i)).

The next lemma shows that the bitstrings listed in (10) all belong to distinct necklaces.

Lemma 9. *Let $(x,y) \in G_n$ be a gluing pair as in* (9)*. Then we have $|P(x^0)| = k(x^0) \geq 8$ and $|P(y^0)| = k(y^0) \geq 4$.*

Note that if $(x,y) = (s_n, s_n')$ then we have $k(x^0) = 4$ and therefore $\langle x^0 \rangle = \langle x^4 \rangle$ and $\langle x^2 \rangle = \langle x^6 \rangle$, so for this case the statement of Lemma 9 would not hold.

Proof. Note that for any $n \geq 4$, the star $x = s_n$ is the only rooted tree with $\lambda(x) = 2$. For any other tree x we have $\lambda(x) \geq 4$ by Lemma 4, so by Lemma 6 (v) we have $k(x^0) = 2\lambda(x) \geq 8$.

For $n \geq 4$, we have $\lambda(y) \geq 2$ for any tree $y \in D_n$ by Lemma 4, so by Lemma 6 (v) we have $k(y^0) = 2\lambda(y) \geq 4$. □

Observe from (10) that

$$C(x,y) := (x^0, x^1, x^6, x^5, y^0, y^1) \tag{12}$$

is a 6-cycle in the middle levels graph M_n. The bit positions flipped along this cycle are

$$\alpha(C(x,y)) := (|u|+4, 2, 3, |u|+4, 2, 3). \tag{13}$$

By Lemma 9 we have that for all $i \geq 0$ the 6-cycle $\sigma^i(C(x,y))$ has the two edges $\sigma^i((x^0,x^1))$, $\sigma^i((x^5,x^6))$ in common with the periodic path $\sigma^i(P(x^0))$, and the edge $\sigma^i((y^0,y^1))$ in common with the periodic path $\sigma^i(P(y^0))$. We refer to these three edges as the *f-edges of* $\sigma^i(C(x,y))$, and we refer to $\sigma^i(C(x,y))$ as a *gluing cycle*. Observe that if $[x] \neq [y]$, then $\langle P(x^0) \rangle$ and $\langle P(y^0) \rangle$ are distinct cycles in the necklace graph N_n by Proposition 7 (i), implying that

$$P(x^0) \bowtie P(y^0) := \Big(x^0, y^1, y^2, \ldots, y^{2\lambda(y)-1}, \sigma^{-\lambda(y)}\big((y^0, x^5, x^4, x^3, x^2, x^1, x^6, x^7, \ldots, x^{2\lambda(x)-1})\big)\Big) \tag{14}$$

is a periodic path in the middle levels graph M_n, and together the $2n+1$ periodic paths $\bigcup_{i\geq 0} \sigma^i(P(x^0) \bowtie P(y^0))$ visit all vertices of $\bigcup_{i \geq 0} \sigma^i(P(x^0) \cup P(y^0))$. To see this, recall that $|P(x^0)| = 2\lambda(x)$, $|P(y^0)| = 2\lambda(y)$, and $\sigma^{\lambda(y)}(y^{2\lambda(y)}) = y^0$ by Proposition 7 (ii). Note that the edge set of $\bigcup_{i\geq 0}\sigma^i(P(x^0)\bowtie P(y^0))$ is the symmetric difference of the edge sets of $\bigcup_{i\geq 0}\sigma^i(P(x^0)\cup P(y^0))$ with the gluing cycles $\bigcup_{i\geq 0}\sigma^i(C(x,y))$. Specifically, the f-edges of the gluing cycles $\sigma^i(C(x,y))$, $i\geq 0$, are removed and replaced by the other edges $\sigma^i((x^1,x^6))$, $\sigma^i((y^0,x^5))$, and $\sigma^i((x^0,y^1))$, for all $i\geq 0$.

In the necklace graph N_n, the symmetric difference of the edge sets of the two cycles $\langle P(x^0)\rangle$ and $\langle P(y^0)\rangle$ with the 6-cycle $\langle C(x,y)\rangle$ is a single cycle on the same vertex set as $\langle P(x^0)\rangle\cup\langle P(y^0)\rangle$.

For all $i\geq 0$, we say that the subpath $\sigma^i((x^1,\ldots,x^5))$ of $\sigma^i(P(x^0))$ is *reversed by* $\sigma^i(C(x,y))$. Moreover, we say that two gluing cycles $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ are *compatible*, if they have no f-edges in common. We also say that $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ are *nested*, if the f-edge $\sigma^i((y^0,y^1))$ of $\sigma^i(C(x,y))$ belongs to the path that is reversed by $\sigma^j(C(\hat{x},\hat{y}))$; see Figure 10. In this case we write $\sigma^i(C(x,y))\gg\sigma^j(C(\hat{x},\hat{y}))$. Lastly, we say that $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ are *interleaved*, if the f-edge $\sigma^j((\hat{x}^0,\hat{x}^1))$ of $\sigma^j(C(\hat{x},\hat{y}))$ belongs to the path that is reversed by $\sigma^i(C(x,y))$.

The following key proposition captures the conditions under which a pair of gluing cycles is compatible, interleaved, or nested, respectively.

Proposition 10. *Let $n\geq 4$ and let $(x,y),(\hat{x},\hat{y})\in G_n$ be two gluing pairs with $[x]\neq[y]$, $[\hat{x}]\neq[\hat{y}]$, and $\{[x],[y]\}\neq\{[\hat{x}],[\hat{y}]\}$. Then for any integers $i,j\geq 0$, the gluing cycles $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ defined in* (12) *have the following properties:*

(i) $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ are compatible.
(ii) $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ are interleaved, if and only if $i=j+2$ and $\hat{x}=\rho^2(x)$.
(iii) $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ are nested, if and only $i=j-1$ and $\hat{x}=\rho^{-1}(y)$.

Two nested gluing cycles as in case (iii) of Proposition 10 can be interpreted as follows: We start at the tree x, pull an edge towards the root to reach the tree $y=\mathrm{pull}(x)$, then perform an inverse tree rotation $\hat{x}=\rho^{-1}(y)$, which makes the previously pulled edge eligible to be pulled again, then pull this edge a second time, reaching the tree $\hat{y}=\mathrm{pull}(\hat{x})$. Consequently, nested gluing cycles occur if and only if the same edge of the underlying plane trees is pulled twice in succession; see Figure 10.

Proof. It suffices to prove the lemma for $i=0$ and arbitrary $j\geq 0$, so for the rest of the proof we assume that $i=0$. We consider the bitstrings $z^k:=f^k(z\,0)$ for all $z\in\{x,y,\hat{x},\hat{y}\}$ and $k\geq 0$.

By Proposition 7 (i) and the assumptions $[x]\neq[y]$ and $[\hat{x}]\neq[\hat{y}]$, each of the 6-cycles $\langle C(x,y)\rangle$ and $\langle C(\hat{x},\hat{y})\rangle$ in N_n connects two distinct cycles of the cycle factor $\mathcal{F}_n$ with each other, and the edges of the 6-cycle given by the f-edges of $C(x,y)$ and $C(\hat{x},\hat{y})$ all lie on one of the cycles from the factor. Consequently, by the assumption that $\{[x],[y]\}\neq\{[\hat{x}],[\hat{y}]\}$, it suffices to verify the following three claims about edges in M_n: (1) If $[x]=[\hat{x}]$, then the edge (x^5,x^6) is distinct from $\sigma^j(\hat{x}^0,\hat{x}^1)$, and the edge (x^0,x^1) is distinct from $\sigma^j(\hat{x}^5,\hat{x}^6)$ for all $j\geq 0$. (2) If $[x]=[\hat{x}]$, then the edge $\sigma^j(\hat{x}^0,\hat{x}^1)$ does not belong to the path $(x^1,\ldots,x^5)$ for any $j\geq 0$, with the only possible exception occuring if $\sigma^{-2}(\hat{x}^0,\hat{x}^1)=(x^4,x^5)$ and $\hat{x}=\rho^2(x)$. (3) If $[y]=[\hat{x}]$, then the edge (y^0,y^1) does not belong to the path $\sigma^j(\hat{x}^0,\ldots,\hat{x}^6)$ for any $j\geq 0$, with the only possible exception occuring if $(y^0,y^1)=\sigma^1(\hat{x}^2,\hat{x}^3)$ and $\hat{x}=\rho^{-1}(y)$.

We begin observing that $\sigma^j(z^k)\in A_n$ for even k and $\sigma^j(z^k)\in B_n$ for odd k and all $j\geq 0$. This immediately implies (1). To prove (2), we first show that $\sigma^j(\hat{x}^0)\neq x^2$. This follows from (11), by observing that $t(\sigma^j(\hat{x}^0))=t(\hat{x}^0)$ and $t(x^2)$ differ in the second bit. From (11) we also see that the condition $t(\sigma^j(\hat{x}^0))=t(\hat{x}^0)=t(x^4)=\rho^2(t(x^0))$ is equivalent to $\hat{x}=\rho^2(x)$. Moreover, from (10) we see that $\ell(\sigma^j(\hat{x}^0))=-j$ and $\ell(x^4)=2$, so $\sigma^j(\hat{x}^0)=x^4$ implies that $j=-2$.

To prove (3), we first show that $y^0\notin\{\sigma^j(\hat{x}^0),\sigma^j(\hat{x}^4)\}$. From (11) we see that $t(y^0)$ and $t(\sigma^j(\hat{x}^0))=t(\hat{x}^0)$ differ in the second and third bit, showing that y^0 is different from $\sigma^j(\hat{x}^0)$.

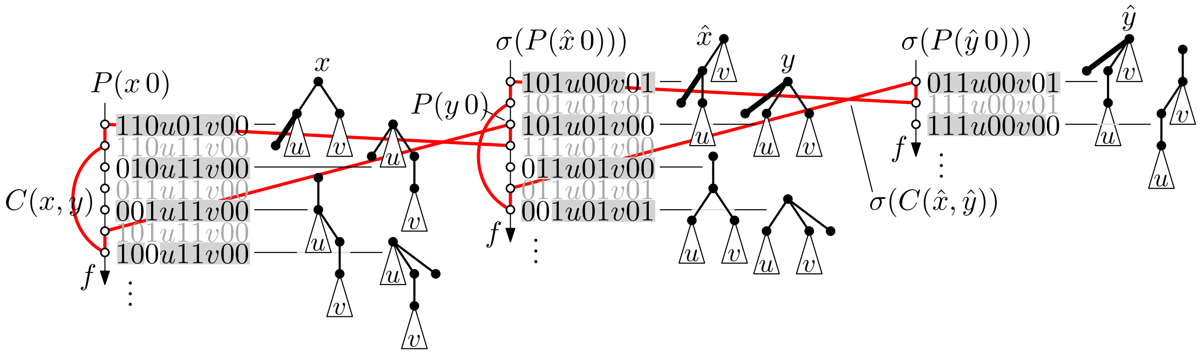


FIGURE 10. Two nested 6-cycles $C(x,y)$ and $C(\hat{x},\hat{y})$. The plane tree $[\hat{y}]$ is obtained from $[x]$ by pulling the same edge twice in succession. This edge is drawn fat in the figure.

From (11) we also obtain that the root of $t(\sigma^j(\hat{x}^4)) = t(\hat{x}^4)$ is a leaf, whereas the root of $t(y^0)$ is not a leaf, proving that y^0 is different from $\sigma^j(\hat{x}^4)$. From the same relation we also see that the condition $t(y^0) = t(\sigma^j(\hat{x}^2)) = t(\hat{x}^2) = \rho(t(\hat{x}^0))$ is equivalent to $y = \rho(\hat{x})$. Moreover, from (10) we see that $\ell(y^0) = 0$ and $\ell(\sigma^j(\hat{x}^2)) = 1 - j$, so $y^0 = \sigma^j(\hat{x}^2)$ implies that $j = 1$.

This completes the proof. □

5. Translation to a spanning tree problem

In this section we combine the ingredients from the previous two sections, and show how they translate Knuth's Gray code problem into the problem of finding a spanning tree $\mathcal{T}_n$ in a suitably defined auxiliary graph $\mathcal{H}_n$, following the ideas outlined in Section 1.6.2. The definitions of the graphs $\mathcal{H}_n$ and $\mathcal{T}_n$ are given in Sections 5.1 and 5.3 below, respectively. Based on this, we describe how flip sequences are glued together inductively along the spanning tree $\mathcal{T}_n$ (Sections 5.4 and 5.5). This allows us to make a first attempt of proving Theorem 1 (Section 5.6). Unfortunately, this attempt does not give a complete proof yet, as we are unable to control the shift value of the flip sequences resulting from the gluing process; recall the discussion from Section 1.6.3. In Section 5.7 we present a method to control the shift value by modifying the spanning tree $\mathcal{T}_n$. With this we are able to prove Theorem 1 for $n \geq 39$ in Section 5.8.

5.1. **Definition of $\mathcal{H}_n$.** For $n \geq 4$, we let $\mathcal{H}_n$ denote the directed arc-labeled multigraph defined as follows: The node set of $\mathcal{H}_n$ is T_n, i.e., all plane trees with n edges. Moreover, for each gluing pair $(x,y) \in G_n$, there is an arc labeled (x,y) from the plane tree $[x]$ to the plane tree $[y]$ in $\mathcal{H}_n$. Some pairs of nodes of $\mathcal{H}_n$ may be connected by multiple arcs oriented the same way (with different labels), such as $([1100110010],[1010110010])$ and $([1100101100],[1010101100])$. Some pairs of nodes may be connected by multiple arcs oriented oppositely, such as $([11010100],[10110100])$ and $([11001010],[10101010])$. There may also be loops in $\mathcal{H}_n$, such as $([11010010],[10110010])$.

Let $\mathcal{T}$ be a simple subgraph of $\mathcal{H}_n$, i.e., $\mathcal{T}$ has no loops and no multiple arcs, neither oriented the same way nor oppositely. We let $G(\mathcal{T})$ be the set of all arc labels of $\mathcal{T}$, i.e., the set of all gluing pairs $(x,y) \in G_n$ that give rise to the arcs in $\mathcal{T}$. As $\mathcal{T}$ is simple, we clearly have $[x] \neq [y]$, $[\hat{x}] \neq [\hat{y}]$, and $\{[x],[y]\} \neq \{[\hat{x}],[\hat{y}]\}$ for all $(x,y),(\hat{x},\hat{y}) \in G(\mathcal{T})$. We say that $G(\mathcal{T})$ is *interleaving-free* or *nesting-free*, respectively, if there are no two gluing pairs $(x,y),(\hat{x},\hat{y}) \in G(\mathcal{T})$ such that the gluing cycles $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ are nested or interleaved for any $i,j \geq 0$.

The next lemma provides a simple sufficient condition guaranteeing interleaving-freeness.

Lemma 11. *If for every gluing pair $(x,y) \in G(\mathcal{T})$, the root of the tree x is not a leaf, then $G(\mathcal{T})$ is interleaving-free.*

Proof. Suppose there are two gluing pairs $(x,y),(\hat{x},\hat{y}) \in G(\mathcal{T})$ such that the gluing cycles $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$ are interleaved for some $i,j \geq 0$. By Proposition 10 (ii), this implies $i = j+2$ and $\hat{x} = \rho^2(x)$. However, note that the root of $\rho^2(x)$ is a leaf (recall (11)), whereas the root of $\hat{x}$ is not a leaf by the assumption of the lemma, so this is a contradiction. □

5.2. **Pullable/pushable leaves.** The following definitions are illustrated in Figure 11. Given a plane tree T and two vertices a,b of T, we let $d(a,b)$ denote the distance of a and b in T, and we let $p^i(a,b)$, $i = 0,1,\ldots,d(a,b)$, be the ith vertex on the path from a to b in T. In particular, we have $p^0(a,b) = a$ and $p^{d(a,b)}(a,b) = b$.

Consider a vertex c and a leaf a of T with $d(a,c) \geq 2$. We say that a is *pullable to* c, if $p(a,c)$ has no neighbors between $p^2(a,c)$ and a in its ccw ordering of neighbors. We say that a is *pushable to* c, if $p(a,c)$ has no neighbors between a and $p^2(a,c)$ in its ccw ordering of neighbors.

Consider a vertex c and a leaf a of T with $d(a,c) \geq 1$. We say that a is *pullable from* c, if $d(a,c) \geq 2$ and $p(a,c)$ has at least one neighbor between $p^2(a,c)$ and a in its ccw ordering of neighbors, of if $d(a,c) = 1$ and c is not a leaf. We say that a is *pushable from* c, if $d(a,c) \geq 2$ and $p(a,c)$ has at least one neighbor between a and $p^2(a,c)$ in its ccw ordering of neighbors, or if $d(a,c) = 1$ and c is not a leaf.

For any odd $n \geq 5$ we define the *dumbbells* $d_n := 1(10)^{(n-1)/2}0(10)^{(n-1)/2} \in D_n$ and $d'_n := \rho^{-2}(d_n) := 101(10)^{(n-1)/2}0(10)^{(n-3)/2} \in D_n$. Each dumbbell has two centroids of degree $(n+1)/2$ each, and all remaining vertices are leaves.

Given a plane tree T with a unique centroid c, we refer to every c-subtree of T as *active*. If T has two centroids c,c', we refer to every c-subtree of T except the one containing c', and to every c'-subtree of T except the one containing c as *active*. Note that if $T \notin \{[s_n],[d_n]\}$, then it has a centroid with an active subtree that is not a single edge.

The following two lemmas describe certain pull/push operations on plane trees that preserve the centroid(s), and that change the tree potential by ± 1.

Lemma 12. *Let c be a centroid of a plane tree T, let a be a leaf of T that is pullable to c, which if $T \neq [d_n]$ belongs to an active c-subtree, and define the rooted tree $x := x(T,c,a) := T^{(a'',a')}$, where $a' := p(a,c)$ and $a'' := p^2(a,c)$. Then x is a pullable tree, the rooted tree $y := \mathrm{pull}(x)$ satisfies $\varphi(y) = \varphi(x) - 1$, and the leaf a is pushable from c in $[y]$. If $x \neq d_n$, then the centroid(s) of x and y are identical and contained in the right subtrees of x and y. If $x = d_n$, then x has two centroids, namely the roots of its left and right subtree, and the root of the right subtree is the unique centroid of y.*

Proof. The statements follow immediately from the definitions given before the lemma, and by Lemma 8. To see that $x \neq s_n$ note that the star $[s_n]$ has a unique centroid c and no leaves that are pullable to c. □

Lemma 13. *Let c be a centroid of a plane tree T, let a be a thick leaf of T that is pushable to c, which if $T \neq [d'_n]$ belongs to an active c-subtree, and define the rooted tree $y := y(T,c,a) := T^{(a',a)}$, where $a' := p(a,c)$. Then y is a pushable tree, the rooted tree $x := \mathrm{push}(y)$ satisfies $\varphi(x) = \varphi(y) - 1$, and the leaf a is pullable from c in $[y]$. If $y \neq d'_n$, then the centroid(s) of y and x are identical and contained in the left subtrees of y and x. If $y = d'_n$, then y has two centroids, namely the roots of its left and right subtree, and the root of the left subtree is the unique centroid of x.*

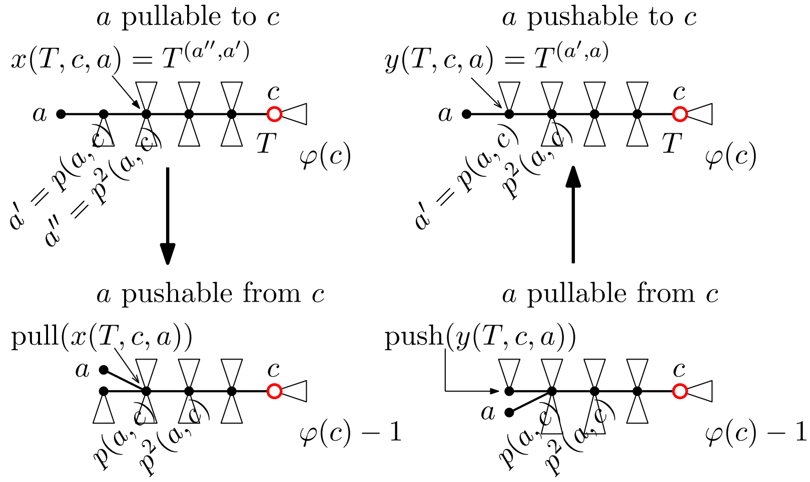


Figure 11. Definition of pullable and pushable leaves.

Proof. The proof is analogous to Lemma 12. To see that $y \neq s'_n$ note that a is assumed to be thick, unlike the leaf we would push in s'_n to obtain s_n. □

5.3. **Definition of $\mathcal{T}_n$.** We define a subgraph $\mathcal{T}_n$ of $\mathcal{H}_n$ as follows: For every plane tree $T \in T_n$ with $T \notin \{[s_n], [d_n]\}$, we fix a vertex c that is a centroid of T and that has at least one active c-subtree that is not a single edge. The leftmost leaf of every such c-subtree is pullable to c. We fix one such leaf a with maximum distance from c. For $T = [d_n]$, we let c be one of its centroids, which has exactly one c-subtree that is not a single edge, namely the tree $s_{(n+1)/2}$. The leftmost leaf a of this subtree is pullable to c. In both cases, let $x := x(T, c, a)$ be the corresponding pullable rooted tree as defined in Lemma 12, and define $y := \mathrm{pull}(x)$, yielding the gluing pair $(x, y) \in G_n$. We let $\mathcal{T}_n$ be the spanning subgraph of $\mathcal{H}_n$ that is given by the union of arcs $([x], [y])$ labeled (x, y) for all gluing pairs (x, y) obtained in this way. In the above definition, ties in the case of two centroids or in the case of multiple leaves with maximum distance from c can be broken arbitrarily.

The next lemma shows that the graph $\mathcal{T}_n$ defined above is indeed a spanning tree of $\mathcal{H}_n$, and moreover the potential of plane trees along every arc of $\mathcal{T}_n$ changes by by -1. For any arc (T, T'), we say that T' is an *out-neighbor* of T, and we say that T is an *in-neighbor* of T'.

Lemma 14. *The graph $\mathcal{T}_n$ is a spanning tree of $\mathcal{H}_n$, and for every arc (T, T') in $\mathcal{T}_n$ we have $\varphi(T') = \varphi(T) - 1$. Every plane tree T other than the star $[s_n]$ has exactly one neighbor T' with $\varphi(T') = \varphi(T) - 1$, which is an out-neighbor. Furthermore, $G(\mathcal{T}_n)$ is interleaving-free.*

Proof. Consider the gluing pair $(x, y) \in G(\mathcal{T}_n)$ added for the plane tree T with $T = [x]$. By Lemma 12 we have $\varphi(y) = \varphi(x) - 1$, i.e., the potential of the trees changes by -1 along every arc of $\mathcal{T}_n$. It follows that in $\mathcal{T}_n$, every plane tree T other than the star $[s_n]$ has exactly one neighbor T' with $\varphi(T') = \varphi(T) - 1$, which is an out-neighbor. Consequently, $\mathcal{T}_n$ has no cycles, regardless of the orientation of arcs along the cycle (in particular, there are no loops). As from every plane tree $T \in T_n$, we can reach a tree T' with $\varphi(T') = \varphi(T) - 1$, there is a directed path from T to the star $[s_n]$, which is the unique plane tree with minimum potential n. We showed that $\mathcal{T}_n$ does not contain cycles and is connected, i.e., it is a spanning tree. By Lemma 12, for any gluing pair $(x, y) \in G(\mathcal{T}_n)$ the right subtree of x contains a centroid of x. As a centroid is never a leaf, the right subtree of x contains edges, i.e., the root of x is not a leaf, so we may apply Lemma 11 to conclude that $G(\mathcal{T}_n)$ is interleaving-free. □

5.4. **Basic operations on flip sequences.** We now describe some basic operations on flip sequences that will be used heavily in the next section when gluing flip sequences together.

Consider a periodic path $P = (x_1, \dots, x_k)$ in the middle levels graph M_n. We say that a sequence of integers $\alpha = (a_1, \dots, a_k)$ is a *flip sequence* for P, if a_i is the position in which x_{i+1} differs from x_i for all $i = 1, \dots, k-1$, and the vertex x_{k+1} obtained from x_k by flipping the bit at position a_k satisfies $\langle x_{k+1} \rangle = \langle x_1 \rangle$. There is unique integer λ modulo $2n+1$ given by the relation $x_1 = \sigma^{\lambda}(x_{k+1})$. We define $\lambda(\alpha) := \lambda$, and we refer to this quantity as the *shift* of α. In words, the parameter λ describes by how much the necklace representatives get rotated to the right when traversing the periodic path once.

We also define

$$\begin{aligned} \operatorname{rev}(P) &:= \Big(x_1, \sigma^{\lambda(\alpha)}\big((x_k, x_{k-1}, \dots, x_2)\big)\Big), \\ \operatorname{rev}(\alpha) &:= (a_k, a_{k-1}, \dots, a_1) - \lambda(\alpha), \end{aligned} \tag{15a}$$

where indices are considered modulo $2n+1$, as always. Note that $\operatorname{rev}(\alpha)$ is a flip sequence for the periodic path $\operatorname{rev}(P)$ satisfying

$$\lambda(\operatorname{rev}(\alpha)) = -\lambda(\alpha). \tag{15b}$$

Given $P = (x_1, \dots, x_k)$ and $\alpha = (a_1, \dots, a_k)$ as before, we define

$$\begin{aligned} \operatorname{mov}(P) &:= (x_2, \dots, x_k, \sigma^{-\lambda(\alpha)}(x_1)), \\ \operatorname{mov}(\alpha) &:= (a_2, \dots, a_k, a_1 + \lambda(\alpha)). \end{aligned} \tag{16a}$$

Note that $\operatorname{mov}(\alpha)$ is a flip sequence for the periodic path $\operatorname{mov}(P)$ satisfying

$$\lambda(\operatorname{mov}(\alpha)) = \lambda(\alpha), \tag{16b}$$

which means that the shift is independent of the choice of the starting vertex along the path. Similarly, for any integer i we have that $\alpha + i$ is a flip sequence for the periodic path $\sigma^{-i}(P)$ satisfying

$$\lambda(\alpha + i) = \lambda(\alpha). \tag{17}$$

For example, the periodic path $P = (1010100, 1110100, 0110100, 0110101)$ has the flip sequence $\alpha = (2, 1, 7, 2)$ with $\lambda(\alpha) = 2$, and the periodic path $\operatorname{rev}(P) = (1010100, 1010101, 1010001, 1010011)$ has the flip sequence $\operatorname{rev}(\alpha) = (7, 5, 6, 7)$ with shift $\lambda(\operatorname{rev}(\alpha)) = -2$. Moreover, $\operatorname{mov}(\alpha) = (1, 7, 2, 4)$ is a flip sequence for the periodic path $\operatorname{mov}(P) = (1110100, 0110100, 0110101, 0010101)$ with $\lambda(\operatorname{mov}(\alpha)) = 2$, and $\alpha + 1 = (3, 2, 1, 3)$ is a flip sequence for the periodic path $\sigma^{-1}(P) = (0101010, 0111010, 0011010, 1011010)$ with $\lambda(\alpha + 1) = 2$.

5.5. **Flip sequences for subtrees of $\mathcal{H}_n$.** Using the notation introduced in the previous section, we now describe how to glue flip sequences of periodic paths together inductively along subtrees of $\mathcal{H}_n$. Ultimately, this will be done for the entire spanning tree $\mathcal{T}_n$. The key problem in this gluing process is to keep track of the shift value of the flip sequences resulting after each step.

For any $x \in A_n \cup B_n$, with $k(x)$ defined in (7), we let $\alpha(x)$ be the sequence of positions in which $f^{i+1}(x)$ differs from $f^i(x)$ for all $i = 0, \dots, k(x) - 1$. Clearly, $\alpha(x)$ is a flip sequence for the periodic path $P(x)$ defined in (8a). By Proposition 7 (ii), we have

$$\lambda(\alpha(x)) = \lambda(t(x)). \tag{18}$$

Let $\mathcal{T}$ be any subtree of $\mathcal{H}_n$ such that $G := G(\mathcal{T})$ is interleaving-free. We define the set of necklaces $N(\mathcal{T}) := \bigcup_{[x] \in \mathcal{T}} \langle P(x\,0) \rangle$. By Proposition 7 (i), this is the set of all necklaces visited by cycles $\langle P(x\,0) \rangle$ in N_n for which the plane tree $[x]$ belongs to $\mathcal{T}$. In the following, for any $z \in N(\mathcal{T})$ and any $x \in z$ we define two periodic paths $\mathcal{P}_G(x) = \{P, P'\}$ with the same starting vertex x in the middle levels graph M_n and flip sequences $\alpha(P)$ and $\alpha(P')$ for these two paths such that $P' = \mathrm{rev}(P)$ and $\alpha(P') = \mathrm{rev}(\alpha(P))$. Moreover, $\langle P\rangle$ and $\langle P'\rangle$ will be oppositely oriented cycles in the necklace graph N_n with vertex set $N(\mathcal{T})$. These definitions proceed inductively as follows:

Base case: If $\mathcal{T} = [x]$ is an isolated node, then we have $G(\mathcal{T}) = \emptyset$. For all $i, j \geq 0$ we define $y := \sigma^j(f^i(x\,0))$. Note that $\alpha(y)$ is a flip sequence for $P(y)$, and so we may define

$$\mathcal{P}_\emptyset(y) := \{P(y), \mathrm{rev}(P(y))\}, \quad \alpha(P(y)) := \alpha(y), \quad \alpha(\mathrm{rev}(P(y))) := \mathrm{rev}(\alpha(y)),$$

with reversals as defined in (15a).

Induction step: For the induction step, we assume that $\mathcal{T}$ has at least two nodes. Consider all gluing pairs $(x, y), (\hat{x}, \hat{y}) \in G(\mathcal{T})$ for which $\sigma^i(C(x, y))$ and $\sigma^j(C(\hat{x}, \hat{y}))$ are nested for some $i, j \geq 0$. By Proposition 10 (iii), this is only possible if $i = j - 1$ and $\hat{x} = \rho^{-1}(y)$. Consequently, the sequences of arcs of $\mathcal{T}$ that are given by such pairs of nested gluing cycles form directed subpaths of $\mathcal{T}$. In particular, there is a gluing pair $(\hat{x}, \hat{y}) \in G(\mathcal{T})$ satisyfing the following property (*): $\sigma^i(C(x, y)) \not\gg \sigma^j(C(\hat{x}, \hat{y}))$ for any $(x, y) \in G(\mathcal{T})$ and $i, j \geq 0$. Consider the subtrees $\mathcal{T}_1$ and $\mathcal{T}_2$ obtained by removing the arc $([\hat{x}], [\hat{y}])$ from $\mathcal{T}$, and consider the sets of gluing pairs $G_1 := G(\mathcal{T}_1)$ and $G_2 := G(\mathcal{T}_2)$. By Proposition 10 (i), by induction, and by property (*), there is a periodic path $P_1 \in \mathcal{P}_{G_1}(\hat{x}\,0) = (x_1, \ldots, x_k)$ that satisfies $(x_1, \ldots, x_7) = (\hat{x}^0, \ldots, \hat{x}^6)$, and a periodic path $P_2 \in \mathcal{P}_{G_2}(\hat{y}\,0) = (y_1, \ldots, y_l)$ that satisfies $(y_1, y_2) = (\hat{y}^0, \hat{y}^1)$. Moreover, there are corresponding flip sequences $\alpha(P_1) =: \alpha_1 = (a_1, \ldots, a_k)$ and $\alpha(P_2) =: \alpha_2 = (b_1, \ldots, b_l)$. We then define the periodic path

$$P_1 \bowtie P_2 := \Big(x_1, y_2, y_3, \ldots, y_l, \sigma^{-\lambda(\alpha(P_2))}((y_1, x_6, x_5, x_4, x_3, x_2, x_7, x_8, \ldots, x_k))\Big) \tag{19}$$

in the middle levels graph M_n (cf. (14)). Together, the $2n+1$ periodic paths $\bigcup_{i\geq 0} \sigma(P_1 \bowtie P_2)$ visit all vertices of $\bigcup_{i\geq 0} \sigma^i(P_1 \cup P_2)$. Moreover, considering the decomposition $\hat{x} = 1\,u\,0\,v$ with $u, v \in D$, we define

$$\alpha_1 \bowtie \alpha_2 := \Big(3, b_2, b_3, \ldots, b_l, ((|u| + 4, a_5, a_4, a_3, a_2, 2, a_7, a_8, \ldots, a_k)) + \lambda(\alpha(P_2))\Big). \tag{20}$$

As $\alpha_1 \bowtie \alpha_2$ is a flip sequence for the periodic path $P_1 \bowtie P_2$ by (13) and (17), we may define

$$\begin{aligned} P' &:= \mathrm{mov}^j(\sigma^i(P_1 \bowtie P_2)), \quad \alpha' := \mathrm{mov}^j(\alpha_1 \bowtie \alpha_2 - i), \\ \mathcal{P}_G(y) &:= \{P', \mathrm{rev}(P')\}, \quad \alpha(P') := \alpha', \quad \alpha(\mathrm{rev}(P')) := \mathrm{rev}(\alpha'). \end{aligned} \tag{21}$$

for all $i, j \geq 0$, where y is the first vertex of the path $\mathrm{mov}^j(\sigma^i(P_1 \bowtie P_2))$. By induction, the sequence of necklaces $\langle P_i\rangle$, $i \in \{1, 2\}$, is a cycle in the necklace graph N_n with vertex set $N(\mathcal{T}_i)$. Consequently, $\langle P'\rangle$ as defined in (21) is a cycle with vertex set $N(\mathcal{T}_1) \cup N(\mathcal{T}_2) = N(\mathcal{T})$, as desired.

Observe from (16b), (17), (20) and (21) that

$$\lambda(\alpha(P')) = \lambda(\alpha(P_1)) + \lambda(\alpha(P_2)).$$

Unrolling this inductive relation using Proposition 7 (i)+(iii), (15b), and (18), we obtain that

$$\lambda(\alpha(P')) = \sum_{T \in \mathcal{T}} \gamma_T \cdot \lambda(T), \tag{22}$$

where the signs $\gamma_T \in \{+1, -1\}$ are determined by which of the gluing cycles $\sigma^i(C(x, y))$ and $\sigma^j(C(\hat{x}, \hat{y}))$ with $(x, y), (\hat{x}, \hat{y}) \in G(\mathcal{T})$, $i, j \geq 0$, are nested.

The relation (22) allows us to compute the shift of flip sequences of periodic paths obtained by the gluing operation $\bowtie$. For example, consider the three periodic paths $P_1 := P(x\,0)$, $P_2 := P(\hat{x}\,0)$, and $P_3 := P(\hat{y}\,0)$ shown in Figure 10, and the corresponding gluing cycles $C(x, y)$ and $C(\hat{x}, \hat{y})$. Note that the gluing cycles $\bigcup_{i\geq 0} \sigma^i(C(x, y))$ join the paths $\bigcup_{i\geq 0} \sigma^i(P_1 \cup P_2)$, and the gluing cycles $\sigma^i(C(\hat{x}, \hat{y}))$ join the paths $\bigcup_{i\geq 0} \sigma^i(P_2 \cup P_3)$. As $\hat{x} = \rho^{-1}(y)$, we have that

$\sigma^i(C(x,y))$ and $\sigma^{i+1}(C(\hat{x},\hat{y}))$ are nested for all $i \geq 0$ by Proposition 10 (iii). For $n=8$, $u=10$ and $v=11101000$ the corresponding flip sequences $\alpha_1 := \alpha(x\,0)$, $\alpha_2 := \alpha(\hat{x}\,0)$, and $\alpha_3 := \alpha(\hat{y}\,0)$ have the shifts $\lambda(\alpha_1) = n = 8$, $\lambda(\alpha_2) = \lambda(\alpha_3) = 2n = 16$ (recall (18)). The 36th and 37th vertices on the periodic path $P_2 \bowtie P_3$ are $\sigma^{-17}(y^1)$ and $\sigma^{-17}(y^0)$, respectively (recall that $y^0 = y\,0$ and $y^1 = f(y^0)$). Consequently, y^0 and y^1 are the first two vertices on the periodic path $P_{23} := \mathrm{rev}(\mathrm{mov}^{36}(\sigma^{17}(P_2 \bowtie P_3)))$ with flip sequence $\alpha_{23} := \mathrm{rev}(\mathrm{mov}^{36}(\alpha_2 \bowtie \alpha_3 - 17))$. The resulting flip sequence $\alpha := \alpha_1 \bowtie \alpha_{23}$ for the periodic path $P := P_1 \bowtie P_{23}$ has shift $\lambda(\alpha) = \lambda(\alpha_1) - \big(\lambda(\alpha_2) + \lambda(\alpha_3)\big) = 8 - (16+16) = -24$.

5.6. **A first attempt at proving Theorem 1.** Let $\mathcal{T}_n$ be the spanning tree of $\mathcal{H}_n$ defined in Section 5.3, i.e., the node set of $\mathcal{T}_n$ is the set T_n of all plane trees with n edges. By Lemma 14, $G(\mathcal{T}_n)$ is interleaving-free. We fix the vertex $x_1 := 1^n 0^{n+1} \in A_n \cup B_n$. The set $\mathcal{P}_{G(\mathcal{T}_n)}(x_1)$ defined in Section 5.5 contains a periodic path P with starting vertex x_1 and second vertex $f(x_1)$ in the middle levels graph M_n such that $\langle P\rangle$ has the vertex set $N(\mathcal{T}_n) = \bigcup_{[x]\in T_n} \langle P(x\,0)\rangle = \{\langle x\rangle \mid x \in A_n \cup B_n\}$, i.e., $\langle P\rangle$ is a Hamilton cycle in the necklace graph N_n. By (22), the corresponding flip sequence $\alpha(P)$ has a shift of

$$\lambda(\alpha(P)) = \sum_{T\in T_n} \gamma_T \cdot \lambda(T) \tag{23}$$

for some signs $\gamma_T \in \{+1,-1\}$ that are determined by which gluing cycles encoded by $\mathcal{T}_n$ are nested.

With $s := \lambda(\alpha(P))$ we define the flip sequences

$$\alpha_0 := \alpha(P), \quad \alpha_i := \alpha_0 + i\cdot s \text{ for } i = 1,\ldots,2n. \tag{24}$$

If we apply the entire flip sequence $(\alpha_0,\alpha_1,\ldots,\alpha_{2n})$ to the starting vertex x_1 in the middle levels graph M_n, then we reach the vertex $\sigma^{-i\cdot s}(x_1)$ after applying all flips in $(\alpha_0,\alpha_1,\ldots,\alpha_{i-1})$ for every $i = 1,\ldots,2n+1$. Consequently, if s and $2n+1$ happen to be coprime, then we reach x_1 only after applying the entire flip sequence, and as $\alpha_0 = \alpha(P)$ is the flip sequence of the Hamilton cycle $\langle P\rangle$ in the necklace graph N_n, the resulting sequence C of bitstrings is a Hamilton cycle in the middle levels graph M_n. A star transposition Gray code for $(n+1,n+1)$-combinations satisfying the conditions of Theorem 1 is then obtained from C by prefixing every bitstring of C with 1 or 0, alternatingly.

However, the aforementioned approach requires that $s = \lambda(\alpha(P))$ and $2n+1$ are coprime, which not be the case. Even if the two numbers were coprime, then this approach only establishes Theorem 1 for one particular value of s, and it is hard to control what this value will be, without further knowledge about the signs γ_T in (23). In particular, if we want to achieve a shift of $s=1$, which is Knuth's original conjecture, then we need a controlled way of modifying $\alpha(P)$ to another flip sequence $\alpha(P')$, so that we obtain a shift of $\lambda(\alpha(P')) = 1$ or any other shift $\lambda(\alpha(P')) = s$ that is coprime to $2n+1$. Given that $\lambda(\alpha(P))$ modulo $2n+1$ could possibly be any number from $\{0,1,\ldots,2n\}$, both tasks are equally difficult. In the next section we show how to accomplish these tasks by carefully modifying the spanning tree $\mathcal{T}_n$ locally.

5.7. **Modifying the spanning tree $\mathcal{T}_n$.** In this section we describe how to locally modify the spanning tree $\mathcal{T}_n$ defined in Section 5.3 before, such that we can control the shift value of the flip sequences that result from the gluing process.

We define the rooted tree $p_\ell := 1^\ell 0^\ell$. This is the path with ℓ edges rooted at one of its end vertices. For any binary vector $\beta = (\beta_1,\ldots,\beta_k) \in \{0,1\}^k$, we define $t_\beta := (p_{\ell_1}, p_{\ell_2}, \ldots, p_{\ell_k})$ with $\ell_i := 2$ if $\beta_i = 0$ and $\ell_i := 3$ if $\beta_i = 1$ for $i = 1,\ldots,k$. In words, t_β is obtained by gluing together k

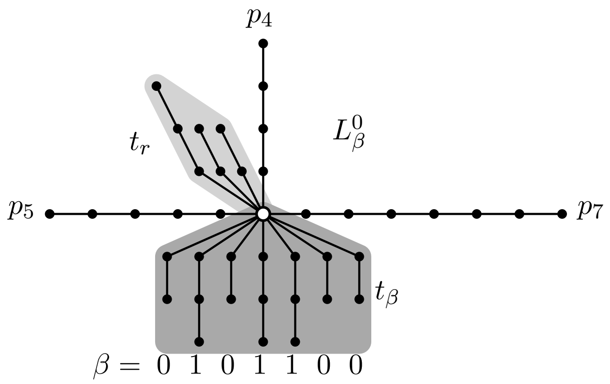


FIGURE 12. Definition of the plane tree L^0_β for $n = 40$, with the centroid highlighted.

paths at their end vertices, a path of length 2 for every 0-bit and a path of length 3 for every 1-bit of β, ordered from left to right at the root of t_β according to the ordering of bits in β. Note that

$$e(t_\beta) = 2k + w(\beta) \leq 3k, \tag{25}$$

where $w(\beta)$ denotes the number of 1s in β.

For any integer $r \geq 2$, we also define $t_r := p_2^{r/2}$ for even r and $t_r := (p_2^{(r-3)/2}, p_3)$ for odd r. Clearly, we have

$$e(t_r) = r. \tag{26}$$

In words, t_r is a tree with r edges that is obtained by gluing together paths of length 2 at their end vertices, possibly adding a path of length 3 as the last path if r is odd.

For a given integer $n \geq 21$, we define

$$k = k(n) := \lfloor n/3 \rfloor - 6 \geq 1, \tag{27}$$

and for any binary vector $\beta \in \{0,1\}^k$, we define

$$r = r(n, \beta) := n - 16 - (2k + w(\beta)). \tag{28}$$

Observe that

$$r \overset{(28),(25)}{\geq} n - 16 - 3k \overset{(27)}{=} n - 16 - 3(\lfloor n/3 \rfloor - 6) = 2 + n - 3\lfloor n/3 \rfloor \geq 2. \tag{29}$$

We then define

$$L^0_\beta := [(t_\beta, p_7, p_4, t_r, p_5)], \tag{30}$$

i.e., L^0_β is the plane tree obtained by gluing together the trees $t_\beta, p_7, p_4, t_r, p_5$ at their roots in ccw order; see Figure 12. We clearly have

$$e(L^0_\beta) = (7 + 4 + 5) + e(t_\beta) + e(t_r) \overset{(25),(26)}{=} 16 + (2k + w(\beta)) + r \overset{(28)}{=} n, \tag{31}$$

i.e., we have $L^0_\beta \in T_n$.

Consider the collections

$$\begin{aligned} L_\beta &:= \{L^0_\beta, L^1_\beta, \widetilde{L}^1_\beta, L^2_\beta, \widetilde{L}^2_\beta, L^3_\beta, \widetilde{L}^3_\beta, L^4_\beta\}, \\ T_\beta &:= \{T^1_\beta, T^2_\beta, \widetilde{T}^2_\beta, T^3_\beta, T^5_\beta\} \end{aligned} \tag{32}$$

of in total 13 distinct plane trees shown in Figure 13, all of which are obtained from L^0_β by modifying only the paths p_7, p_4, p_5 in the definition (30), by suitably replacing them by trees with the same number of edges (7, 4, or 5, respectively), as shown in the figure. We refer to these three subtrees as the *arms* of each $T \in L_\beta \cup T_\beta$. In Figure 13, the subtrees t_β and t_r that are the same in each tree are indicated by gray-shaded areas. We also consider the following pairs of trees from the set L_β

$$\begin{aligned}&\mathcal{C}_\beta := \{(L_\beta^0, L_\beta^1), (L_\beta^1, L_\beta^2), (L_\beta^2, L_\beta^3), (L_\beta^3, L_\beta^4), (L_\beta^0, \widetilde{L}_\beta^1), (\widetilde{L}_\beta^1, \widetilde{L}_\beta^2), (\widetilde{L}_\beta^2, \widetilde{L}_\beta^3), (\widetilde{L}_\beta^3, L_\beta^4)\},\\ &\mathcal{L}_\beta := \mathcal{C}_\beta \cup \{(L_\beta^4, T_\beta^5)\}.\end{aligned} \tag{33a}$$

These are the pairs of trees joined by solid arcs in Figure 13. We also define the following two subsets of $\mathcal{L}_\beta$

$$\begin{aligned}\mathcal{C}_\beta^+ &:= \mathcal{C}_\beta \setminus \{(L_\beta^0, \widetilde{L}_\beta^1)\}, \quad \mathcal{C}_\beta^- := \mathcal{C}_\beta \setminus \{(L_\beta^0, L_\beta^1)\},\\ \mathcal{L}_\beta^+ &:= \mathcal{L}_\beta \setminus \{(L_\beta^0, \widetilde{L}_\beta^1)\}, \quad \mathcal{L}_\beta^- := \mathcal{L}_\beta \setminus \{(L_\beta^0, L_\beta^1)\}.\end{aligned} \tag{33b}$$

We will show that $\mathcal{C}_\beta$ and $\mathcal{L}_\beta$ are subgraphs of $\mathcal{H}_n$ that span the set of nodes L_β or $L_\beta \cup \{T_\beta^5\}$, respectively. In fact, $\mathcal{C}_\beta$ is a cycle, and $\mathcal{L}_\beta$ is a cycle with a pending edge attached to it, and we refer to it as a *lollipop*. Moreover, $\mathcal{L}_\beta^+$ and $\mathcal{L}_\beta^-$ are two distinct spanning trees of the lollipop $\mathcal{L}_\beta$.

The next proposition captures all key properties of the lollipop subgraphs $\mathcal{L}_\beta$ of $\mathcal{H}_n$ that will be needed later on. In particular, property (vi) asserts that switching between the two distinct spanning trees $\mathcal{L}_\beta^+$ and $\mathcal{L}_\beta^-$ of $\mathcal{L}_\beta$ changes the shift value of a flip sequence by $-4n$, which is crucial. This is achieved by making $G(\mathcal{L}_\beta)$ nesting-free, except for the arcs $(L_\beta^0, \widetilde{L}_\beta^1)$ and $(\widetilde{L}_\beta^1, \widetilde{L}_\beta^2)$, which are both present in $\mathcal{L}_\beta^-$, but not in $\mathcal{L}_\beta^+$.

Proposition 15. *For $n \geq 21$ and k as defined in* (27) *we have the following:*

(i) For any $\beta \in \{0,1\}^k$ and any plane tree T from one of the sets L_β or T_β defined in (32)*, the unique vertex with degree at least 5 is the centroid of T.*

(ii) For any $\beta \in \{0,1\}^k$ and any plane tree $T \in L_\beta \cup T_\beta$, we have $\lambda(T) = 2n$.

(iii) For distinct binary vectors $\beta, \beta' \in \{0,1\}^k$, the sets of trees $L_\beta \cup T_\beta$ and $L_{\beta'} \cup T_{\beta'}$ are disjoint.

(iv) For any $\beta \in \{0,1\}^k$, the spanning tree $\mathcal{T}_n$ defined in Section 5.3 *has no arcs (T, T') or (T', T) with $\varphi(T') = \varphi(T) - 1$ and $T \notin L_\beta$ and $T' \in L_\beta$.*

(v) For any $\beta \in \{0,1\}^k$ and for every pair (T, T') of trees from $\mathcal{L}_\beta$ defined in (33a)*, there is a unique gluing pair $(x, y) \in G_n$ with $([x],[y]) = (T, T')$. Consequently, the lollipop $\mathcal{L}_\beta$ is a subgraph of $\mathcal{H}_n$ that spans the set of nodes $L_\beta \cup \{T_\beta^5\}$, and $\mathcal{L}_\beta^+$ and $\mathcal{L}_\beta^-$ defined in* (33b) *are spanning trees of $\mathcal{L}_\beta$. Moreover, $G(\mathcal{L}_\beta^+)$ is interleaving-free and nesting-free, and $G(\mathcal{L}_\beta^-)$ is interleaving-free and nesting-free, except for the two gluing pairs $(x, y), (\hat{x}, \hat{y}) \in G(\mathcal{L}_\beta^-)$ that are given by $([x],[y]) = (L_\beta^0, \widetilde{L}_\beta^1)$ and $([\hat{x}],[\hat{y}]) = (\widetilde{L}_\beta^1, \widetilde{L}_\beta^2)$, which satisfy $\sigma^i(C(x,y)) \gg \sigma^{i+1}(C(\hat{x},\hat{y}))$ for all $i \geq 0$.*

(vi) Consider the subtrees $\mathcal{C}_\beta^+$ and $\mathcal{C}_\beta^-$ of $\mathcal{H}_n$ defined in (33) *that span the set of nodes L_β, and define $G^+ := G(\mathcal{C}_\beta^+)$ and $G^- := G(\mathcal{C}_\beta^-)$. Moreover, let $(x, y) \in G_n$ be the gluing pair with $([x],[y]) = (L_\beta^4, T_\beta^5)$. Also, let P^+ be the periodic path from $\mathcal{P}_{G^+}(x\,0)$ defined in Section* 5.5 *that starts with the vertices $x\,0, f(x\,0), \ldots$, and let P^- be the periodic path from $\mathcal{P}_{G^-}(x\,0)$ that starts with the vertices $x\,0, f(x\,0), \ldots$. Then the flip sequences $\alpha(P^+)$ and $\alpha(P^-)$ have shifts $\lambda(\alpha^+) = 2n \cdot 7 + 2n$ and $\lambda(\alpha^-) = 2n \cdot 7 - 2n$.*

The periodic paths P^+ and P^- referred to in (vi) are well-defined, as by (v), $G(\mathcal{C}_\beta^+) \subseteq G(\mathcal{L}_\beta^+)$ and $G(\mathcal{C}_\beta^-) \subseteq G(\mathcal{L}_\beta^-)$ are interleaving-free.

Proof. (i) The trees t_β and t_r in the definition (30) have at least one edge by (27) and (29), and so T has a unique vertex c with degree at least 5 (each of the three arms contributes +1 to the degree of c). Let a be any of the neighbors of c in T. Note that $e(T^{(a,c)--}) \geq 4 + 5 = 9$, and $e(T^{(c,a)--}) \leq 7 - 1 = 6$, as the smaller two of the three arms of T have at least 4 and 5 edges,

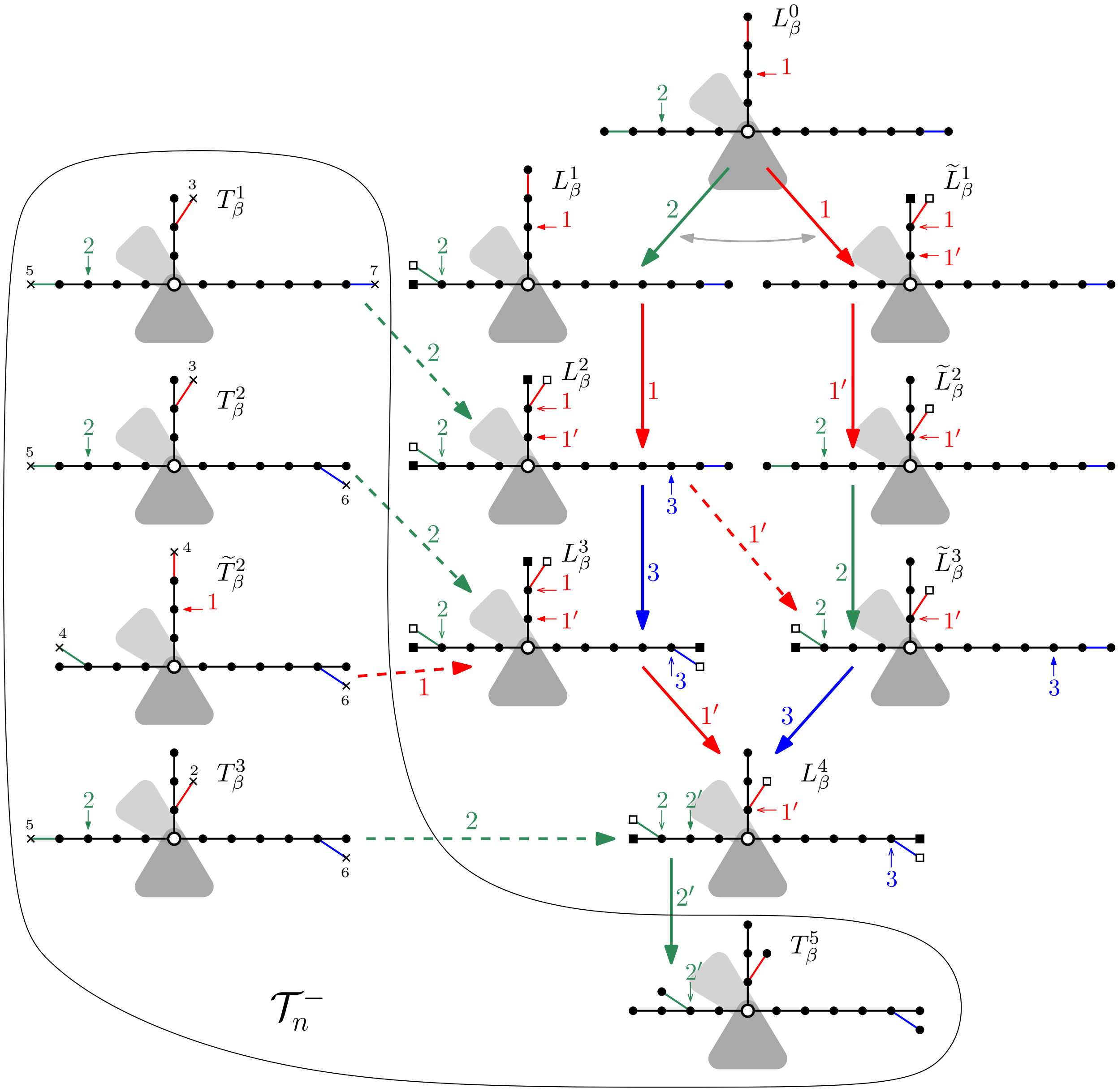


FIGURE 13. Definition of the families of plane trees L_β and T_β. In each tree, the centroid c is marked with a white bullet. Leaves of the trees in L_β that are pushable from c or pullable from c are marked with a white square or black square, respectively. Leaves of the trees in $T_\beta \setminus \{T^5_\beta\}$ that are pullable to c are marked with a cross, with a small number next to them indicating the distance to the centroid. Large solid arrows show the arcs of the lollipop subgraph $\mathcal{L}_\beta$ of $\mathcal{H}_n$. Large dashed arrows show arcs of the graph $\mathcal{H}_n$, which are not present in $\mathcal{T}_n$, however. In $\mathcal{H}_n$, every arc $([x],[y])$ is labeled with a gluing pair (x,y), and in the figure, the rooted trees x and y are obtained by rooting the plane trees $[x]$ and $[y]$ at the vertices indicated by the small arrows, which also show the splitting of the cyclic ordering of neighbors of this vertex to obtain the left-to-right ordering of the children of the root. For clarity, every arc (large arrow) and the corresponding two small arrows are marked by the same integer. The large gray double arrow indicates two arcs, exactly one of which is in $\mathcal{L}^+_\beta$ and the other one is in $\mathcal{L}^-_\beta$.

respectively, and the largest of the three arms of T has at most 7 edges. Applying Lemma 3, we obtain that $\varphi(a) - \varphi(c) \geq 9 - 6 > 0$, proving that c must be the unique centroid.

(ii) Consider the centroid c of T given by (i), and consider the cyclic ordering of subtrees around c. Due to the presence of the three arms with 7, 4, or 5 edges, respectively, this sequence of trees has no cyclic symmetries, implying that $\lambda(T) = 2n$, as $e(T) = n$ (recall (31)).

(iii) This follows by observing that the binary vector β can be recovered uniquely from each tree $T \in L_\beta \cup T_\beta$. Indeed, T has a unique vertex c of degree at least 5. Moreover, there is a unique subtree with 5 edges emanating from c, which is the second-largest of the three arms. The next subtrees emanating from c in ccw direction are paths of length 2 or 3, which encode the binary vector β. This sequence of subtrees is terminated by a subtree with 7 edges emanating from c, which is the largest of the three arms of T.

(iv) By Lemma 14, along every arc (T, T') of $\mathcal{T}_n$ we have $\varphi(T') = \varphi(T) - 1$, so it is enough to prove that $\mathcal{T}_n$ has no arcs (T, T') from a node $T \notin L_\beta$ to a node $T' \in L_\beta$. For any $T' \in L_\beta$, let c be its centroid given by (i). By Lemma 12, every incoming arc at T' corresponds to a leaf of T' that is pushable from c. As all leaves have distance at least 2 from c in T', any leaf that is pushable from c is thick by definition, so we need to consider only thick leaves of T'. In particular, the trees t_β and t_r in the definition (30) have only thin leaves, and therefore contain no leaves pushable from c. Only the three arms of T' have thick leaves, and may therefore have leaves pushable from c. All leaves of trees $T' \in L_\beta$ that are pushable from c are marked by a white square in Figure 13. In particular, L_β^0 has no leaves that are pushable from c, and therefore no incoming arcs in $\mathcal{T}_n \subseteq \mathcal{H}_n$. L_β^1 and $\widetilde{L}_\beta^1$ have one leaf each that is pushable from c, coming from the arcs (L_β^0, L_β^1) and $(L_\beta^0, \widetilde{L}_\beta^1)$, respectively, which we can ignore as their starting nodes are in L_β. The tree L_β^2 has two leaves that are pushable from c, one from the arc (L_β^1, L_β^2), which we can ignore. The second one comes from the arc (T_β^1, L_β^2) of $\mathcal{H}_n$, which however, is not present in $\mathcal{T}_n$, by the choice of a leaf in T_β^1 that is pullable to c and that has maximum distance from the centroid in the definition of $\mathcal{T}_n$. All leaves of trees $T' \in T_\beta \setminus \{T_\beta^5\}$ that are pullable to c are marked by crosses in Figure 13, with their distance from the centroid indicated next to them. The tree $\widetilde{L}_\beta^2$ has one leaf that is pushable from c coming from the arc $(\widetilde{L}_\beta^1, \widetilde{L}_\beta^2)$, which we can ignore. The tree L_β^3 has three leaves that are pushable from c, one from the arc (L_β^2, L_β^3), which we can ignore, and two from the arcs (T_β^2, L_β^3) and $(\widetilde{T}_\beta^2, L_\beta^3)$ of $\mathcal{H}_n$, which are not present in $\mathcal{T}_n$, by the choice of leaf in T_β^2 and $\widetilde{T}_\beta^2$ that is pullable to c and that has maximum distance from the centroid. The tree $\widetilde{L}_\beta^3$ has two leaves that are pushable from c from the arcs $(L_\beta^2, \widetilde{L}_\beta^3)$ and $(\widetilde{L}_\beta^2, \widetilde{L}_\beta^3)$, which we can both ignore. Finally, the tree L_β^4 has three leaves that are pushable from c, two from the arcs (L_β^3, L_β^4) and $(\widetilde{L}_\beta^3, L_\beta^4)$, which we can ignore, and one from the arc (T_β^3, L_β^4), which is not present in $\mathcal{T}_n$, by the choice of a pullable leaf in T_β^3 that is pullable to c and that has maximum distance from the centroid.

(v) Figure 13 shows how to root the plane trees T, T' of each pair $(T, T') \in \mathcal{L}_\beta$, such that the rooted trees x, y with $(T, T') = ([x], [y])$ form a gluing pair $(x, y) \in G_n$. In the figure, every pair $(T, T') \in \mathcal{L}_\beta$ is joined by a large solid arrow marked by $j = 1, 1', 2, 2', 3$, and the small arrows marked j next to T and T' indicate the root vertex, and the splitting of the cyclic ordering of neighbors of this vertex to obtain the left-to-right ordering of the children of the root. One can check that the resulting pairs of rooted trees (x, y) have the form (9), i.e., $y = \mathrm{pull}(x)$, and consequently these are indeed gluing pairs in G_n. Moreover, none of the tree vertices marked as root is a leaf, implying that $G(\mathcal{L}_\beta^+)$ and $G(\mathcal{L}_\beta^-)$ are interleaving-free by Lemma 11.

Using Proposition 10 (iii), one can check that no two of the gluing cycles $\sigma^i(C(x,y))$, with $(x,y) \in G(\mathcal{L}_\beta)$ and $i \geq 0$, are nested, except for the cycles $\sigma^i(C(x,y)) \gg \sigma^{i+1}(C(\hat{x},\hat{y}))$, $i \geq 0$, that are given by $([x],[y]) = (L_\beta^0, \widetilde{L}_\beta^1)$ and $([\hat{x}],[\hat{y}]) = (\widetilde{L}_\beta^1, \widetilde{L}_\beta^2)$. This is because in any two pull operations corresponding to two consecutive arcs of the lollipop $\mathcal{L}_\beta$, we never pull the same tree edge twice in succession, except in the latter case.

(vi) By (22), we need to evaluate the sums $\sum_{T\in L_\beta} \gamma_T \cdot \lambda(T)$ for both sets of gluing pairs G^+ and G^-. By (ii), we have $\lambda(T) = 2n$ for each of the eight trees $T \in L_\beta$. Moreover, from (v) we obtain that $G(\mathcal{C}_\beta^+) \subseteq G(\mathcal{L}_\beta^+)$ is nesting-free and therefore we have $\gamma_T = +1$ for each of the eight trees $T \in L_\beta$, showing that $\alpha(P^+) = 2n \cdot 8 = 2n \cdot 7 + 2n$. On the other hand, $G(\mathcal{C}_\beta^-) \subseteq G(\mathcal{L}_\beta^-)$ is nesting-free except for the gluing pairs $(x,y), (\hat{x},\hat{y}) \in G(\mathcal{C}_\beta^-)$ that are given by $([x],[y]) = (L_\beta^0, \widetilde{L}_\beta^1)$ and $([\hat{x}],[\hat{y}]) = (\widetilde{L}_\beta^1, \widetilde{L}_\beta^2)$, which satisfy $\sigma^i(C(x,y)) \gg \sigma^{i+1}(C(\hat{x},\hat{y}))$ for all $i \geq 0$. As L_β^0 is a leaf of $\mathcal{C}_\beta^-$, we obtain that $\gamma_{L_\beta^0} = -1$ and $\gamma(T) = +1$ for all $T \in L_\beta \setminus \{L_\beta^0\}$. Consequently, we obtain that $\alpha(P^-) = 2n \cdot 7 - 2n$.

This completes the proof. □

5.8. **Proof of Theorem 1 for $n \geq 39$.** We are now in position to prove Theorem 1 for all sufficiently large values of n.

Proof of Theorem 1 for $n \geq 39$. Let $n \geq 39$, let k be as defined in (27), and let $\mathcal{T}_n$ be the spanning tree of $\mathcal{H}_n$ defined in Section 5.3. The following definitions are illustrated in Figure 14. Let $\mathcal{T}_n^-$ denote the subgraph of $\mathcal{T}_n$ obtained by removing all nodes in the sets L_β defined in (32) for all $\beta \in \{0,1\}^k$. From Lemma 14 we know that every node T of $\mathcal{T}_n$ has at most one neighbor T' with $\varphi(T') = \varphi(T) - 1$. Combining this with Proposition 15 (iv) shows that $\mathcal{T}_n^-$ is still a connected graph. We now extend $\mathcal{T}_n^-$ to a spanning tree of $\mathcal{H}_n$, by adding all arcs from either the set $\mathcal{L}_\beta^+$ or $\mathcal{L}_\beta^-$ as defined in (33) for all $\beta \in \{0,1\}^k$. This choice for each $\beta \in \{0,1\}^k$ is encoded in a sign sequence χ of length 2^k, and the entries of this sequence are indexed by β, so $\chi_\beta \in \{+,-\}$ for all $\beta \in \{0,1\}^k$. As each of $\mathcal{L}_\beta^+$ and $\mathcal{L}_\beta^-$ is a spanning tree on the same set of nodes $L_\beta \cup \{T_\beta^5\}$ by Proposition 15 (v), and as these sets of nodes are disjoint for distinct binary vectors $\beta, \beta' \in \{0,1\}^k$ by Proposition 15 (iii),

$$\mathcal{T}_n(\chi) := \mathcal{T}_n^- \cup \bigcup_{\beta\in\{0,1\}^k} \mathcal{L}_\beta^{\chi_\beta} \tag{34}$$

is a spanning tree of $\mathcal{H}_n$ for every sign sequence χ. Each of the subtrees $\mathcal{L}_\beta^{\chi_\beta} \subseteq \mathcal{L}_\beta$ is connected to $\mathcal{T}_n^-$ via the node T_β^5, which is the end node of the 'handle' of the lollipop $\mathcal{L}_\beta$.

For each such spanning tree, we can now define a periodic path $P(\chi)$ in the middle levels graph M_n as described in Section 5.6, and by (23) and (34), the shift of the corresponding flip sequence $\alpha(P(\chi))$ is

$$\lambda(\alpha(P(\chi))) = \underbrace{\sum_{T\in\mathcal{T}_n^-} \gamma_T \cdot \lambda(T)}_{=:\lambda_0} + \sum_{\beta\in\{0,1\}^k} \underbrace{\sum_{T\in L_\beta} \gamma_T \cdot \lambda(T)}_{=:\lambda_\beta} \tag{35}$$

for some signs $\gamma_T \in \{+1,-1\}$. Note that the first summand λ_0 in (35) is a fixed integer that is independent of χ, as the tree $\mathcal{T}_n^-$ is independent of χ. Moreover, the inner sum λ_β of the second summand in (35) is $\gamma_\beta(2n \cdot 7 + 2n)$ if $\chi_\beta = +$ or $\gamma_\beta(2n \cdot 7 - 2n)$ if $\chi_\beta = -$ by Proposition 15 (vi), where $\gamma_\beta \in \{+1,-1\}$. Therefore, by choosing $\chi_\beta \in \{+,-\}$ appropriately, we can change the value of the shift $\lambda(\alpha(P(\chi)))$ by $-4n$. Note that $-4n = 2$ modulo $2n+1$, and that 2 and $2n+1$ are coprime. Therefore, to make the sum (35) modulo $2n+1$ have any possible value s in $\{0,1,\ldots,2n\}$, it is enough if we have at least $2n$ choices for β, i.e., if $2^k \geq 2n$ (for proving the theorem we

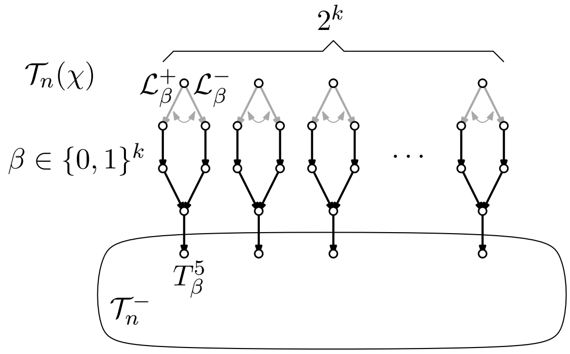


FIGURE 14. Definition of the tree $\mathcal{T}_n(\chi)$. Each node represents a plane tree from T_n, as shown in Figure 13, which provides a zoomed view of a single lollipop $\mathcal{L}_\beta$. The double arrows show the choice between two arcs that we may remove from the lollipop $\mathcal{L}_\beta$ to obtain the subtrees $\mathcal{L}^+_\beta$ and $\mathcal{L}^-_\beta$, for each binary vector $\beta \in \{0,1\}^k$. Each such choice changes the shift of the resulting flip sequence by $-4n = 2 \pmod{2n+1}$.

would only need values of s that are coprime to $2n+1$). From the definition (27) we see that this inequality holds for all $n \geq 39$. At this point the construction of the flip sequence satisfying the conditions of Theorem 1 proceeds as explained in Section 5.6 with the definition (24). □

6. Redefining the spanning tree

The proof of Theorem 1 for $n \geq 39$ presented in Section 5.8 fails for $n \leq 38$, as there are not enough lollipops $\mathcal{L}_\beta$ available to adjust the shift of the resulting flip sequence in (35) to any value $s \in \{0, 1, \ldots, 2n\}$ that is coprime to $2n+1$. Recall that we have essentially no control over the value of λ_0 in (35), as the signs $\gamma_T \in \{+1, -1\}$ depend on which pairs of gluing cycles $\sigma^i(C(x,y))$ and $\sigma^j(C(\hat{x},\hat{y}))$, $i, j \geq 0$, with gluing pairs $(x,y), (\hat{x},\hat{y}) \in G(\mathcal{T}_n)$ are nested. For some small values of n, we could of course compute the value of λ_0 explicitly, but this takes exponential time and space, given that the number of plane trees in T_n is exponential. This seems feasible maybe for $n \leq 20$, but certainly not for $n \geq 30$ (note that $|T_{30}| \geq 10^{13}$). So for some small values of n we do not know λ_0, and even if we knew the value, the methods presented so far do not allow us to adjust the value to the desired shift s.

The problem of not knowing the value of λ_0 is also a fundamental obstacle in translating the proof presented before to an efficient algorithm for computing the corresponding Gray code for any n. Specifically, if the algorithm does not not know λ_0, then it first has to compute its value, to be able to adjust it to the desired shift s, or to any shift s that is coprime to $2n+1$. However, this would take exponential time and space for initialization, which is inacceptable.

There is one obvious idea that solves both problems simultaneously: If we construct a spanning tree $\mathcal{T}_n$ of $\mathcal{H}_n$ such that $G(\mathcal{T}_n)$ is not only interleaving-free, but also *nesting-free*, then all signs γ_T in (35) are positive, which allows us to use the closed form expression

$$\sum_{T \in T_n} \lambda(T) = C_n, \tag{36}$$

where C_n is the nth Catalan number. To see this identity, recall that $\lambda(T)$ counts all rooted trees whose underlying plane tree is T, so overall we count all rooted trees, which gives the sum $|D_n| = C_n$.

Combining (35), (36), and Proposition 15 (ii) shows that

$$\lambda_0 = C_n - 2^k \cdot 8 \cdot 2n$$

(recall from (32) that $|L_\beta| = 8$), i.e., we have a closed formula for λ_0, which can be computed efficiently. In particular, we only need to compute this number modulo $2n+1$, so all arithmetic deals with small numbers only.

From Lemma 14 we know that for the spanning tree $\mathcal{T}_n$ of $\mathcal{H}_n$ defined in Section 5.3, $G(\mathcal{T}_n)$ is interleaving-free. Unfortunately, $G(\mathcal{T}_n)$ is not nesting-free in general. Consequently, to implement the approach outlined before, in the following we define another spanning tree $\mathcal{T}_n$ of $\mathcal{H}_n$ such that $G(\mathcal{T}_n)$ is both interleaving-free and nesting-free (see Lemma 17 below). This alternative definition of $\mathcal{T}_n$ is considerably more complicated than the one presented in Section 5.3, which is why we deferred it to this point, to separate it clearly from the the other ingredients of the proof (presented in Sections 5.4, 5.5, and 5.7), which will work the same way as before also for the new $\mathcal{T}_n$.

6.1. **Redefinition of $\mathcal{T}_n$.** We define the rooted trees

$$\begin{aligned} &q_0 := 10, && q_1 := 1100, && q_2 := 110100, && q_3 := 11100100, \\ &q_4 := 11010100, && q_5 := 1110100100, && q_6 := 1110010100, && q_7 := 1110011000, \\ &q_8 := 1101011000, && q_9 := 1101010100, \end{aligned} \tag{37}$$

see Figure 15.

We define a subgraph $\mathcal{T}_n$ of $\mathcal{H}_n$, $n \geq 4$, as follows: For every plane tree $T \in T_n$ with $T \neq [s_n]$, we define a gluing pair $(x, y) \in G_n$ with either $T = [x]$ or $T = [y]$. We let $\mathcal{T}_n$ be the spanning subgraph of $\mathcal{H}_n$ given by the union of arcs $([x], [y])$ labeled (x, y) for all gluing pairs (x, y) obtained in this way. The definition of the gluing pair $(x, y) \in G_n$ for a given plane tree $T \neq [d_n]$ proceeds in the following three steps (T1)–(T3), whereas if $T = [d_n]$, then the special rule (D) is applied.

(D) Dumbbell rule. If $T = [d_n]$, we let c be one of its centroids, which has exactly one c-subtree that is not a single edge, namely the tree $s_{(n+1)/2}$. The rightmost leaf a of it is thick and pushable to c in T, so we define $y := y(T, c, a) = d'_n$ and $x := \text{push}(y)$ as in Lemma 13.

(T1) Fix the centroid and subtree ordering. If T has two centroids, we let c denote the centroid whose active c-subtrees are not all single edges. If this is true for both centroids, we let c be the one for which all active c-subtrees $t_1, \ldots, t_k$, listed in ccw order such that t_1 is the first tree encountered after the c-subtree containing the other centroid, give the lexicographically minimal string $(t_1, \ldots, t_k)$.

If T has a unique centroid, we denote it by c. We consider all c-subtrees of T, and we denote them by $t_1, \ldots, t_k$, i.e., $T = [(t_1, \ldots, t_k)]$, such that among all possible ccw orderings of subtrees around c, the string $(t_1, t_2, \ldots, t_k)$ is lexicographically minimal.

(T2) Select c-subtree of T. If T has two centroids, we let $t_{\hat{\imath}}$ be the first of the trees $t_1, \ldots, t_k$ that is distinct from q_0.

If T has a unique centroid, then for each of the following conditions (i)–(v), we consider all trees t_i for $i = 1, \ldots, k$, and we determine the first tree t_i satisfying the condition, i.e., we only check one of these conditions once all trees failed all previous conditions:

(i) t_i has 7 edges,
(ii) $t_i = q_1$ and $t_{i-1} = q_0$,
(iii) $t_i \in \{q_2, q_4\}$ and $t_{i+1} \in \{q_0, q_1, q_2\}$,
(iv) $t_i \notin \{q_0, q_1, q_2, q_4\}$,
(v) $t_i \neq q_0$.

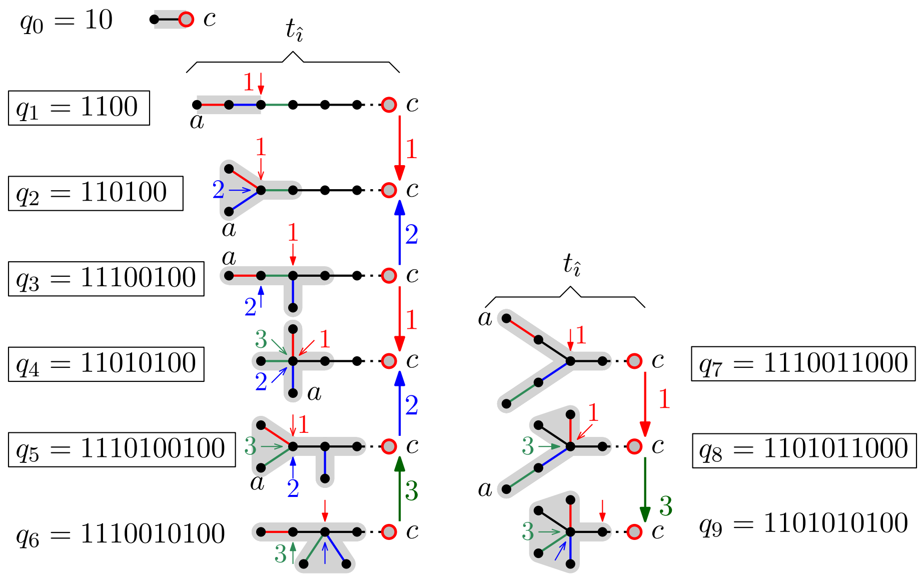


FIGURE 15. Illustration of the trees $q_0, \ldots, q_9$ defined in (37), which are highlighted in gray, and pull/push operations between them. In the spanning tree $\mathcal{T}_n$, every arc $([x], [y])$ is labeled with a gluing pair (x, y), and in the figure, the rooted trees x and y are obtained by rooting the plane trees $[x]$ and $[y]$ at the vertices indicated by the small arrows, which also show the splitting of the cyclic ordering of neighbors of this vertex to obtain the left-to-right ordering of the children of the root. For clarity, every arc and the corresponding two small arrows are marked by the same integer. The framed trees $\{q_1, \ldots, q_5\} \cup \{q_7, q_8\}$ are treated by separate rules in step (T2).

Conditions (ii) and (iii) refer to the previous tree t_{i-1} and the next tree t_{i+1} in the ccw ordering of c-subtrees, and those indices are considered modulo k. Note that T is not the star $[s_n]$, and so at least one c-subtree of T is distinct from q_0 and satisfies the last condition, so this rule to determine t_i is well-defined. We let $t_{\hat{\imath}}$ be the c-subtree determined in this way. Clearly, $t_{\hat{\imath}}$ has at least two edges.

(T3) Select leaf to pull/push. If $t_{\hat{\imath}} = 1^l q_j 0^l$ for some $l \geq 0$ and $j \in \{1, \ldots, 5\} \cup \{7, 8\}$, i.e., $t_{\hat{\imath}}$ is a path with one of the trees $q_1, \ldots, q_5$ or q_7, q_8 attached to it, then we distinguish four cases; see Figure 15:

(q137) If $j \in \{1, 3, 7\}$, then we let a be the leftmost leaf of $t_{\hat{\imath}}$, which is thin, and define $x := x(T, c, a)$ and $y := \mathrm{pull}(x)$ as in Lemma 12. Clearly, for $j = 1$ we have $y = 1^{l-1} q_2 0^{l-1}$ if $l > 0$ and $y = q_0^2$ if $l = 0$, for $j = 3$ we have $y = 1^l q_4 0^l$, and for $j = 7$ we have $y = 1^l q_8 0^l$.

(q24) If $j \in \{2, 4\}$, then we let a be the rightmost leaf of $t_{\hat{\imath}}$, which is thick, and we define $y := y(T, c, a)$ and $x := \mathrm{push}(y)$ as in Lemma 13. Clearly, for $j = 2$ we have $x = 1^{l-1} q_3 0^{l-1}$ if $l > 0$ and $x = q_1 q_0$ if $l = 0$, and for $j = 4$ we have $x = 1^{l-1} q_5 0^{l-1}$ if $l > 0$ and $x = q_2 q_0$ if $l = 0$.

(q5) If $j = 5$, then we let a be unique leaf of $t_{\hat{\imath}}$ that is neither the leftmost nor the rightmost one, which is thick, and we define $y := y(T, c, a)$ and $x := \mathrm{push}(x)$ as in Lemma 13. We clearly have $x = 1^l q_6 0^l$.

(q8) If $j = 8$, then we let a be the rightmost leaf of $t_{\hat{\imath}}$, which is thin, and define $x := x(T, c, a)$ and $y := \mathrm{pull}(x)$ as in Lemma 12. We clearly have $y = 1^l q_9 0^l$.

Otherwise we distinguish two cases:

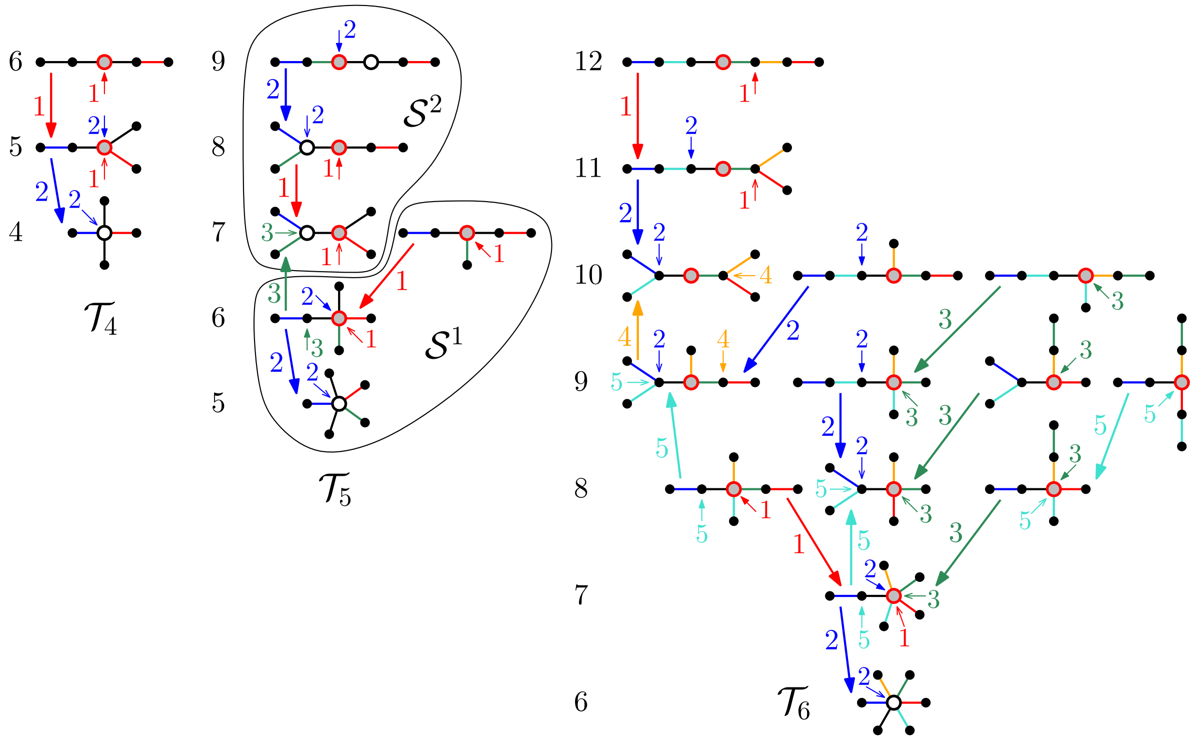


FIGURE 16. Illustration of the spanning trees $\mathcal{T}_4, \mathcal{T}_5, \mathcal{T}_6$. The subgraphs $\mathcal{S}^1, \mathcal{S}^2 \subseteq \mathcal{T}_n$ with all plane trees that have one or two centroids, respectively, are highlighted. Centroid(s) are marked with bullets, where the centroid selected in step (T1) is filled gray. Plane trees are arranged in levels according to their potential, which is shown on the side. The arrow markings are explained in Figure 15.

(e) If the potential $\varphi(T) = \varphi(c)$ is even, we let a be the leftmost leaf of $t_{\hat{\imath}}$ and define $x := x(T, c, a)$ and $y := \mathrm{pull}(x)$ as in Lemma 12.

(o1) If the potential $\varphi(T) = \varphi(c)$ is odd and the rightmost leaf a of $t_{\hat{\imath}}$ is thin, we define $x := x(T, c, a)$ and $y := \mathrm{pull}(x)$ as in Lemma 12.

(o2) If the potential $\varphi(T) = \varphi(c)$ is odd and the rightmost leaf a of $t_{\hat{\imath}}$ is thick, we define $y := y(T, c, a)$ and $x := \mathrm{push}(y)$ as in Lemma 13.

This completes the definition of $\mathcal{T}_n$. In Lemma 17 below we will show that $\mathcal{T}_n$ is indeed a spanning tree of $\mathcal{H}_n$. The spanning trees $\mathcal{T}_n \subseteq \mathcal{H}_n$ for $n = 4, 5, 6, 7$ are shown in Figures 16 and 17.

In the following, we refer to rules (q137), (q8), (e), and (o1) in step (T3) as *pull rules*, and to rules (q24), (q5), and (o2) as *push rules*. Note that the leaf to which one of the pull rules (q137), (q8) or (o1) is applied, is always thin, whereas the leaf to which any push rule is applied, is always thick.

6.2. **Properties of $\mathcal{T}_n$.** The main task of this section is to prove that $\mathcal{T}_n$ is a spanning tree of $\mathcal{H}_n$ for which $G(\mathcal{T}_n)$ is interleaving-free and nesting-free (Lemma 17 below). The following lemma is an auxiliary statement that will be used in that proof.

Lemma 16. *If T has a unique centroid c, then the c-subtree $t_{\hat{\imath}}$ selected in step (T2) satisfies the following conditions:*

(a) If $t_{\hat{\imath}} = q_1$, then $t_{\hat{\imath}-1} = q_0$ or $t_1 = t_2 = \cdots = t_k = q_1$.
(b) If $t_{\hat{\imath}} \in \{q_2, q_4\}$, then $t_{\hat{\imath}+1} \in \{q_0, q_1, q_2\}$ or $t_1 = t_2 = \cdots = t_k = q_4$.

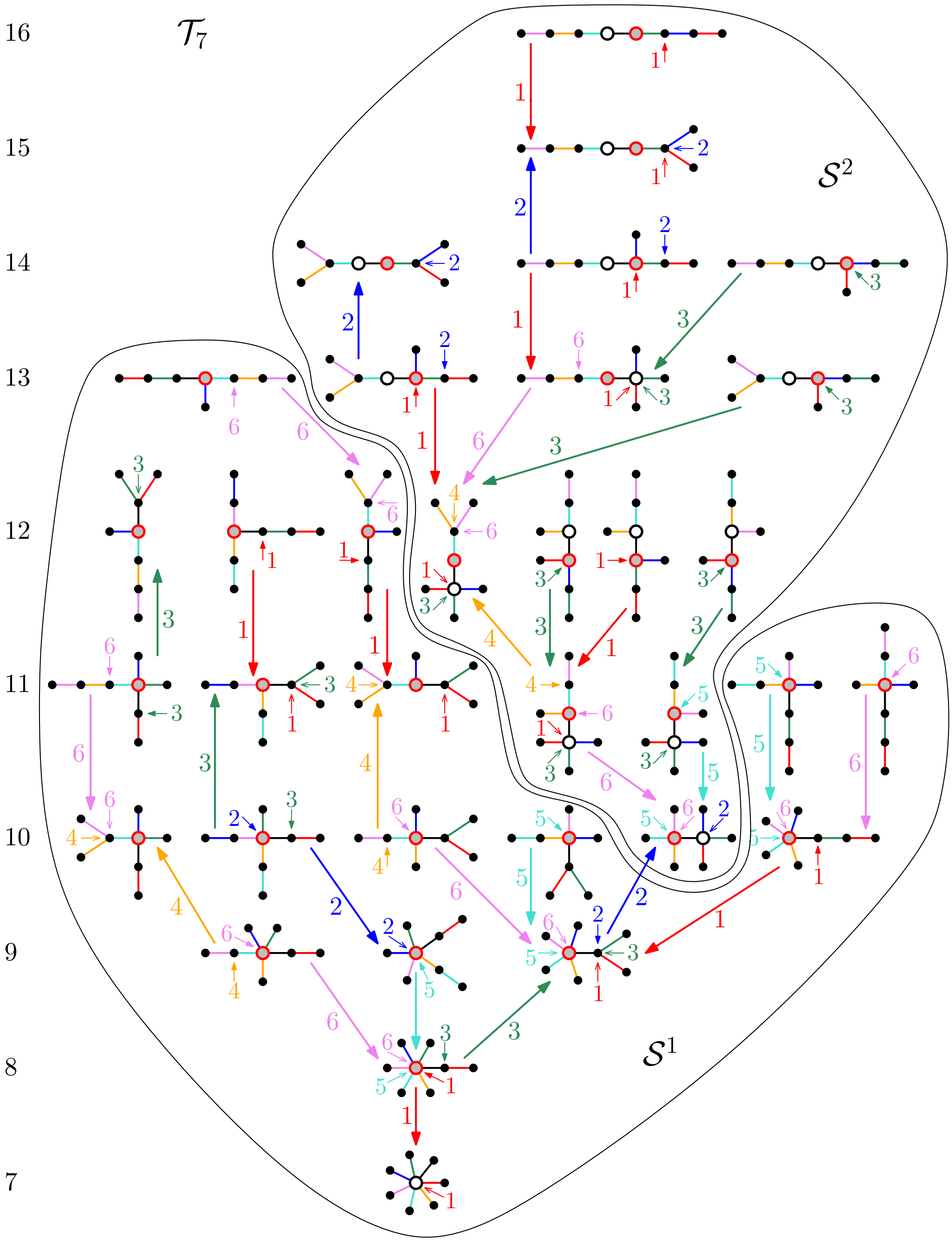


FIGURE 17. Illustration of the spanning tree $\mathcal{T}_7$. Notation is as in Figure 15.

Proof. We first prove (a). Among the conditions (i)–(v) that are checked in step (T2), only conditions (ii) and (v) lead to selecting a c-subtree that is isomorphic to q_1 for $t_{\hat{\imath}}$. If condition (ii) holds, then we clearly have $t_{\hat{\imath}-1} = q_0$ by (i). If condition (v) applies, then all c-subtrees $t_1, \ldots, t_k$ of T failed all previous conditions (i)–(iv). In particular, from (ii) we know that $t_i = q_1$ implies that $t_{i-1} \neq q_0$. Moreover, from (iii) we obtain that $t_{i-1} \notin \{q_2, q_4\}$. Combining this with (iv) shows that $t_{i-1} = q_1$. This proves part (a) of the lemma.

It remains to prove part (b). Among the conditions (i)-(v), only conditions (iii) and (v) lead to selecting a c-subtree that is isomorphic to q_2 or q_4 for $t_{\hat{\imath}}$. If condition (iii) holds, then we clearly have $t_{\hat{\imath}+1} \in \{q_0, q_1, q_2\}$. If condition (v) applies, then all c-subtrees $t_1, \ldots, t_k$ of T failed all previous conditions (i)–(iv). In particular, from (iii) we know that $t_i \in \{q_2, q_4\}$ implies that $t_{i+1} \notin \{q_0, q_1, q_2\}$. Combining this with (iv) shows that $t_{i+1} = q_4$. This proves part (b) of the lemma. □

Lemma 17. *The graph $\mathcal{T}_n$ is a spanning tree of $\mathcal{H}_n$, and for every arc (T, T') in $\mathcal{T}_n$ we either have $\varphi(T') = \varphi(T) - 1$ or $\varphi(T) = \varphi(T') - 1$. Every plane tree T other than the star $[s_n]$ has exactly one neighbor T' with $\varphi(T') = \varphi(T) - 1$, which is an out-neighbor or in-neighbor. Furthermore, $G(\mathcal{T}_n)$ is interleaving-free and nesting-free.*

Proof. Consider a gluing pair $(x, y) \in G(\mathcal{T}_n)$ added for a plane tree T with $T = [x]$. By Lemma 12 we have $\varphi(y) = \varphi(x) - 1$, i.e., the potential of the trees changes by -1 along this arc. On the other hand, consider a gluing pair (x, y) added for a plane tree T with $T = [y]$. By Lemma 13 we have $\varphi(x) = \varphi(y) - 1$, i.e., the potential of the trees changes by $+1$ along this arc. It follows that in $\mathcal{T}_n$, every plane tree T other than the star has exactly one neighbor T' with $\varphi(T') = \varphi(T) - 1$, which is an out-neighbor or in-neighbor. Consequently, $\mathcal{T}_n$ has no cycles, regardless of the orientation of arcs along the cycle (in particular, there are no loops). As from every plane tree $T \in T_n$, we can reach a tree T' with $\varphi(T') = \varphi(T) - 1$, there is a path from T to the star $[s_n]$, which is the unique plane tree with minimum potential n. We showed that $\mathcal{T}_n$ does not contain cycles and is connected, i.e., it is a spanning tree.

We now show that $G(\mathcal{T}_n)$ is interleaving-free. By Lemma 12, for any gluing pair $(x, y) \in G(\mathcal{T}_n)$ with $\varphi(y) = \varphi(x) - 1$ the right subtree of x contains a centroid of x. As a centroid is never a leaf, the right subtree of x contains edges, i.e., the root of x is not a leaf. For any gluing pair $(x, y) \in G(\mathcal{T}_n)$ with $\varphi(x) = \varphi(y) - 1$, as y is obtained from x by a push rule, the pushed leaf in y is thick, i.e., the right subtrees of y and x contain edges, and hence the root of x is not a leaf. We can thus apply Lemma 11 to conclude that $G(\mathcal{T}_n)$ is interleaving-free.

The remainder of the proof is devoted to showing that $G(\mathcal{T}_n)$ is nesting-free.

We let $\mathcal{S}^1$ and $\mathcal{S}^2$ denote the subgraphs of $\mathcal{T}_n$ induced by all plane trees with a unique centroid, or with two centroids, respectively. By Lemma 3, $\mathcal{S}^1 = \mathcal{T}_n$ and $\mathcal{S}^2 = \emptyset$ for even n, whereas $\mathcal{S}^1$ and $\mathcal{S}^2$ are both nonempty for odd n; see Figures 16 and 17. For any plane tree $T \neq [s_n]$ in $\mathcal{T}_n$, consider the tree T' with $\varphi(T') = \varphi(T) - 1$ that is connected to T in $\mathcal{T}_n$. By Lemmas 12 and 13, if T has a unique centroid, then T' also has a unique centroid. Similarly, if T has two centroids, then T' also has two centroids, except if $T = [d_n] = [d'_n]$, in which case $T' = [\mathrm{push}(d'_n)]$ has a unique centroid. Consequently, $\mathcal{S}^1$ and $\mathcal{S}^2$ are subtrees of $\mathcal{T}_n$, with only a single arc between them, namely the arc $([\mathrm{push}(d'_n)], [d'_n])$.

The following arguments are illustrated in Figure 18. Suppose for the sake of contradiction that $G(\mathcal{T}_n)$ is not nesting-free. Then by Proposition 10 (iii), there are gluing pairs $(x, y), (\hat{x}, \hat{y}) \in G(\mathcal{T}_n)$ with $\hat{x} = \rho^{-1}(y)$. We consider the plane trees $T := [\hat{x}] = [y]$, $T' := [\hat{y}]$, and $T'' := [x]$. We let a denote the leaf in which $\hat{x}$ and $\hat{y}$ differ, which is also the leaf in which x and y differ. Moreover, we let b denote the root of $\hat{x}$, b' the root of y, and b'' the leftmost child of the root of x. As $\hat{x}$ and x are pullable trees, we have $\hat{x} = 1\,1\,0\,u'\,0\,w$ and $x = 1\,1\,0\,u\,0\,v'$ for $u', w, u, v' \in D$ (recall (9)). Combining these relations with $\hat{x} = \rho^{-1}(y)$ shows that if $u' = \varepsilon$, then we have $u = w$ and $v' = \varepsilon$ (in particular, $b = b''$), whereas if $u' \neq \varepsilon$, then we have $u' = 1\,u\,0\,v$ and $v' = v\,1\,w\,0$. The vertex identifiers a, b, b', b'' and the subtree identifiers u, v, w apply to the rooted trees $x, y, \hat{x}, \hat{y}$, but also to the plane trees T, T', T''. Note that $\hat{x} = T^{(b,b')}$, $y = T^{(b',a)}$,

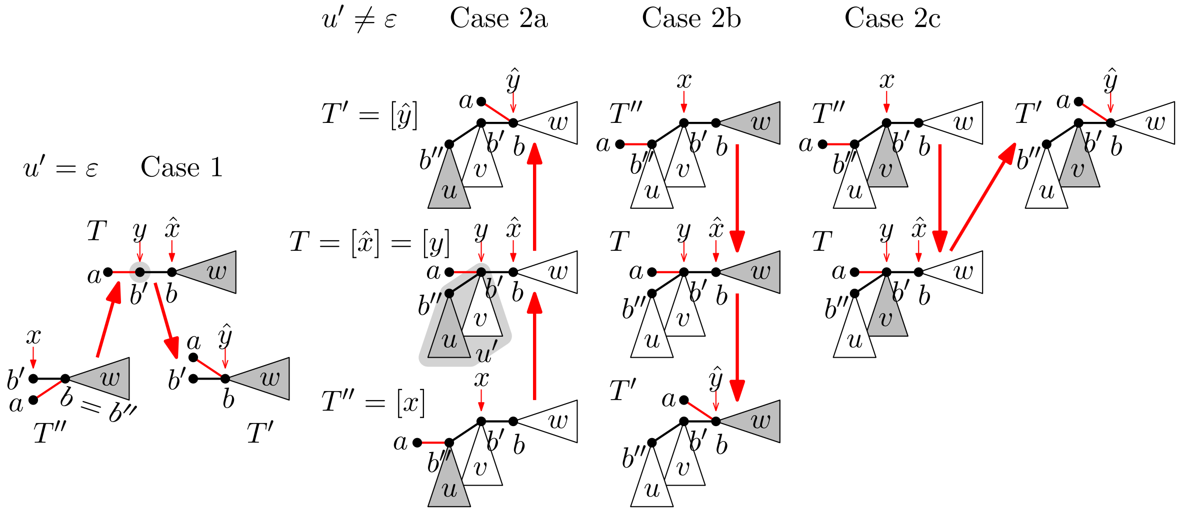


FIGURE 18. Notations used in the proof that $G(\mathcal{T}_n)$ is nesting-free. The gray subtrees contain the centroid(s).

$\hat{y} = T'^{(b,a)}$, and $x = T''^{(b',b'')}$. We let c, c', c'' denote the centroid of T, T', T'', respectively, selected in step (D) or (T1), and we let t, t', t'' denote the subtrees selected in step (D) or (T2).

Case 1: We first consider the case $u' = \varepsilon$. In this case the leaf a of $T = [\hat{x}] = [y]$ is thin, and so both $T' = [\hat{y}] = [\text{pull}(\hat{x})]$ and $T'' = [x] = [\text{push}(y)]$ have smaller potential than T, i.e., we have $\varphi(T') = \varphi(T'') = \varphi(T) - 1$. This is impossible however, as T has only a single neighbor in $\mathcal{T}_n$ with potential $\varphi(T) - 1$.

We now consider the case $u' \neq \varepsilon$.

Case 2a: $\varphi(T') = \varphi(T) + 1$ and $\varphi(T'') = \varphi(T) - 1$. In this case, the leaf a is thick and pushable to c' in T', implying that $w \neq \varepsilon$, and the leaf a is thick and pushable to c in T.

Subcase 2a(i): $T, T', T'' \in \mathcal{S}^1$ or $T, T', T'' \in \mathcal{S}^2$. By Lemmas 12 and 13, the centroid(s) of T, T', T'' are identical. As a is pushable to c and in an active c-subtree in T, the centroid(s) of T are in u, in particular, c is in u. As a is in an active c'-subtree of T', we must have $c' = c$.

As $\hat{x}$ is obtained from $\hat{y}$ by a push applied to the leaf a, one of the push rules (q24), (q5) or (o2) in step (T3) applies to t' in T'.

However, rule (q5) does not apply, as the rightmost leaf of q_5 is missing in t'.

If rule (q24) applies to t', i.e., t' is a path with q_2 or q_4 attached to it (in particular, $v = \varepsilon$), then t is a path with q_3 or q_5 attached to it, respectively, i.e., rule (q137) or (q5) apply to t in T. However, rule (q137) is a pull rule, not a push rule, a contradiction. If rule (q5) applies to t, then this rule applies a push to a leaf in w, but not to a, a contradiction.

If rule (o2) applies to t' in T', i.e., $\varphi(T')$ is odd and a is the rightmost leaf of t', then $\varphi(T) = \varphi(T') - 1$ is even, so rule (o2) does not apply to t in T. It remains to check that none of the push rules (q24) or (q5) applies to t, either. Rule (q5) does not apply, as the rule does not push a, which is the rightmost leaf of t, but rather a leaf that is neither the rightmost nor the leftmost leaf of t. Rule (q24) does not apply either, as $w \neq \varepsilon$. In each case, we arrive at a contradiction.

Subcase 2a(ii): $T = [d_n] \in \mathcal{S}^2$ and $T'' = [\text{push}(d_n')] \in \mathcal{S}^1$. By rule (D), it suffices to consider the case that the centroids of T are b' and b'' and $c = b''$, i.e., we have $u = q_0^{(n-1)/2}$, $v = q_0^{(n-5)/2}$, and $w = \varepsilon$. Then we have $c' = b'$ and rule (q137) of step (T3) applies to the c'-subtree $1w100 = 1100 = q_1$ of T', but this is a pull rule, not a push rule, a contradiction.

Subcase 2a(iii): $T' = [d_n] \in \mathcal{S}^2$ and $T = [\text{push}(d_n')] \in \mathcal{S}^1$. By rule (D), it suffices to consider the case that the centroids of T' are b and b' and $c' = b'$, i.e., we have $u = \varepsilon$ and $v = w = q_0^{(n-3)/2}$. Then $c = b'$ is the unique centroid of T, and the leaf a is not pushable to c in T, a contradiction.

Case 2b: $\varphi(T'') = \varphi(T) + 1$ and $\varphi(T') = \varphi(T) - 1$. In this case, the leaf a is pullable to c'' in T'', and the leaf a is thick (due to the vertex b'') and pullable to c in T.

Subcase 2b(i): $T, T', T'' \in \mathcal{S}^1$ or $T, T', T'' \in \mathcal{S}^2$. By Lemmas 12 and 13, the centroid(s) of T, T', T'' are identical. As a is pullable to c and in an active c-subtree in T, the centroid(s) of T are in w, in particular, c is in w. As a is in an active c''-subtree of T'', we must have $c'' = c$.

As y is obtained from x by a pull applied to the leaf a, one of the pull rules (q137), (q8), (e) or (o1) in step (T3) applies to t'' in T''.

However, rule (q8) does not apply, as the leftmost leaf of q_8 is missing in t''.

If rule (q137) applies to t'', i.e., t'' is a path with q_1, q_3, or q_7 attached to it (in particular, $u = \varepsilon$), then t is a path with q_2, q_4, or q_8 attached to it, respectively, i.e., rule (q24) or (q8) apply to t in T. However, rule (q24) is a push rule, not a pull rule, a contradiction. Also, rule (q8) applies a pull to a leaf in v, but not to a, a contradiction.

If rule (e) applies to t'' in T'', i.e., $\varphi(T'')$ is even and a is the leftmost leaf of t'', then $\varphi(T) = \varphi(T'') - 1$ is odd, so rule (e) does not apply to t in T. As a is not the rightmost leaf of t in T due to the edge (b', b''), rule (o1) does not apply to t, either. Moreover, none of the remaining pull rules (q137) or (q8) apply to t, as they only apply to thin leaves, whereas a is thick in T. We arrive at a contradiction.

If rule (o1) applies to t'' in T'', i.e., $\varphi(T'')$ is odd and a is the rightmost leaf of t'', then $\varphi(T) = \varphi(T'') - 1$ is even, so rule (o1) does not apply to t in T. None of the pull rules (q137) or (q8) apply to t due to the fact that a is thick in T, as argued before. Suppose that rule (e) applies to t in T, i.e., a is the leftmost leaf of t. However, if a is the rightmost leaf of t'' and the leftmost leaf of t, then as $c'' = c$ we obtain that t is a path with q_2 attached to it, in which case the push rule (q24) applies to t, a contradiction.

Subcase 2b(ii): $T'' = [d_n]$ or $T = [d_n]$. These cases are impossible as the tree $[d_n]$ has an incoming arc from the tree $[\text{push}(d_n')]$ with lower potential that it is connected to in $\mathcal{T}_n$, and no outgoing arcs to any such tree.

Case 2c: $\varphi(T') = \varphi(T'') = \varphi(T) + 1$. In this case, the leaf a is pullable to c'' in T'', and the leaf a is thick and pushable to c' in T'.

Subcase 2c(i): $T, T', T'' \in \mathcal{S}^1$ or $T, T', T'' \in \mathcal{S}^2$. By Lemmas 12 and 13, the centroid(s) of T, T', T'' are identical. As a is pullable to c'' and in an active c''-subtree in T'', the centroid(s) of T'' are in v or w. Moreover, as a is pushable to c' in T' and in an active c'-subtree of T', the centroid(s) of T' are in v or u. Combining these observations shows that the centroid(s) are in v and $c' = c''$. As y is obtained from x by a pull applied to the leaf a, one of the pull rules (q137), (q8), (e) or (o1) in step (T3) applies to t'' in T''.

In the following we first assume that the centroid is unique, i.e., $T, T', T'' \in \mathcal{S}^1$, and subsequently we explain how to modify these arguments if $T, T', T'' \in \mathcal{S}^2$.

If rule (q137) applies to t'', then due to the edge (b', b), we must have $u = \varepsilon$, $c'' = b'$, and $t'' = q_1$. Using Lemma 16 (a), it follows that $w = \varepsilon$, or n is even and all c''-subtrees of T'' are copies of q_1. In the first case, the leaf a of T' is thin, a contradiction. In the second case, we have $w = q_0$ and $v = q_1^{(n-4)/2}$. If $n = 4$, then b is the unique centroid of T', and not $c' = b'$, a contradiction. If $n \geq 6$, then v consists of at least one copy of q_1, and in T', rule (ii) in step (T2) applies to the c'-subtree given by the leftmost such copy (as $u = \varepsilon$), and this rule has higher priority than rule (iii) that selects the c'-subtree $1w100 = 110100 = q_2$, a contradiction.

If rule (q8) applies to t'' in T'', i.e., t'' is a path with q_8 attached to it, then we have $w=\varepsilon$, i.e., a is thin in T', a contradiction.

If rule (e) applies to t'' in T'', i.e., $\varphi(T'')$ is even and a is the leftmost leaf of t'', then for a to be leftmost in t'', we must have $c''=b'$ due to the edge (b',b). Also we have $u\notin\{\varepsilon,q_0,q_0^2\}$, otherwise the c''-subtree $110u0$ would be equal to q_1,q_2, or q_4, respectively, and then rule (q137) or (q24) would apply to t'' instead of rule (e). Clearly, the push rule (o2) does not apply to t' in T', as $\varphi(T')=\varphi(T'')$ is even. The push rule (q5) does not apply to t' either, as this rule would apply a pull to a leaf in w, and not to a. If the push rule (q24) applies to t', then we have $1w100\in\{q_2,q_4\}$, i.e., $w=q_0$ or $w=q_0^2$. By Lemma 16 (b), the ccw next c'-subtree of $1w100$ in T', namely the tree $1u0$, is from $\{q_0,q_1,q_2\}$, or n is a multiple of 4 and all c'-subtrees of T' are isomorphic to q_4. In the first case, we get $u\in\{\varepsilon,q_0,q_0^2\}$, a contradiction to the conditions on u derived before. In the second case, we have $w=q_0^2$, i.e., the c''-subtree $1w0$ of T'' is isomorphic to q_2. Moreover, we have $u=q_0^3$, and v consists of $(n-8)/4$ copies of q_4. If $n=8$, then $v=\varepsilon$ and the unique centroid of T'' is b'', not $c''=b'$, a contradiction. If $n\geq 12$, then the rightmost copy of q_4 in v has $1w0=q_2$ as its ccw next c''-subtree, implying that rule (iii) in step (T2) applies to this subtree. However, the c''-subtree $t''=110u0=1101010100$ has 5 edges and is distinct from q_0,q_1,q_2,q_4, so it was selected by rule (iv), which has lower priority, a contradiction.

If rule (o1) applies to t'' in T'', i.e., $\varphi(T'')$ is odd and a is the rightmost leaf of t'', then we have $u=\varepsilon$. Moreover, we have $c''\neq b'$, as otherwise rule (q137) would apply to t'' instead of rule (o1), i.e., the centroid of T'' is in v, but not at the root of this subtree. Consequently, the push rule (o2) does not apply to t' in T', as a is not the rightmost leaf of t' due to the edge (b',b''). The push rule (q24) does not apply to t' either, again due to the edge (b',b''), which is missing in q_2 and q_4. If the push rule (q5) applies to t', i.e., t' is a path with q_5 attached to it, then we have $u=\varepsilon$, $w=q_0$ and t'' is a path with q_7 attached to it. However, then rule (q7) applies to t'' in T'', and not rule (o1), a contradiction.

If $T,T',T''\in\mathcal{S}^2$, then the above four cases for the pull rules applied to t'' in T'' can be adapted as follows: The cases where rule (q8) or (o1) applies to t'' are the same, only the cases where the rule (q137) or (e) applies have to be modified, due to the usage of Lemma 16, which only applies if the centroid is unique.

If rule (q137) or (e) applies to t'', then we have $c''=b'$ as before. Now $w=\varepsilon$ follows from the fact that in step (T2), t'' is selected as the first active c''-subtree in ccw order that is not a single edge. But then a is thin in T', a contradiction.

Subcase 2c(ii): $T'=[d_n]\in\mathcal{S}^2$ and $T=[\mathrm{push}(d'_n)]\in\mathcal{S}^1$. By rule (D), it suffices to consider the case that the centroids of T' are b and b' and $c'=b'$, i.e., we have $u=\varepsilon$ and $v=w=(10)^{(n-3)/2}$. Then $c''=b'$ is the unique centroid of T'', and we have $11u0=1100=q_1$. However, this c''-subtree violates the conditions of Lemma 16 (a), as $w\neq\varepsilon$ and v contains at least one c''-subtree that is a single edge, by the assumption $n\geq 4$.

This completes the proof. □

7. Switches

In this section we develop another systematic way to modify the shift value of flip sequences, which works *without modifying the spanning tree* $\mathcal{T}_n$, following the ideas outlined in Section 1.6.3. This will allow us to prove Theorem 1 for $n\leq 38$.

For two bitstrings that differ in a single bit, we write $p(x,y)$ for the position in which x and y differ. We say that a triple of vertices $\tau=(x,y,y')$ with $x\in A_n$, $y,y'\in B_n$ and $y\neq y'$ is a *switch*, if x differs from both y and from y' in a single bit, and $\langle y\rangle=\langle y'\rangle$. In the necklace graph N_n, a switch can be considered as a multiedge $(\langle x\rangle,\langle y\rangle)=(\langle x\rangle,\langle y'\rangle)$. The *shift* of a switch $\tau = (x, y, y')$, denoted $\lambda(\tau)$, is defined as the integer i such that $y = \sigma^i(y')$. For example $\tau = (1110000, 1110001, 1111000)$ is a switch, as we have $\langle 1110001\rangle = \langle 1111000\rangle$, and its shift is $\lambda(\tau) = 1$, as $1110001 = \sigma^1(1111000)$. We denote a switch $\tau = (x, y, y')$ compactly by writing x with the 0-bit at position $p(x, y)$ underlined, and the 0-bit at position $p(x, y')$ overlined. The switch τ from before is denoted compactly as $\tau = 111\overline{0}00\underline{0}$. Note that for any switch $\tau = (x, y, y')$, the inverted switch $\tau^{-1} := (x, y', y)$ has shift $\lambda(\tau^{-1}) = -\lambda(\tau)$. For example, for $\tau = 111\overline{0}00\underline{0}$, the switch $\tau^{-1} = 111\underline{0}00\overline{0}$ has shift $\lambda(\tau^{-1}) = -1$. Clearly, cyclically rotating a switch yields another switch with the same shift. Similarly, reversing a switch yields another switch with the negated shift. For example, the switch $\sigma(\tau) = 11\overline{0}00\underline{0}1$ has shift $+1$, and its reversed switch $1\underline{0}00\overline{0}11$ has shift -1.

7.1. **Modifying flip sequences by switches.** The idea of a switch $\tau = (x, y, y')$ is simple and yet very powerful: Consider a flip sequence $\alpha = (a_1, \ldots, a_k)$ with shift $\lambda(\alpha)$ for a periodic path $P = (x_1, \ldots, x_k)$, and let x_{k+1} be the vertex obtained from x_k by flipping the bit at position a_k. If we have $(x_i, x_{i+1}) = (x, y)$ for some $i \in \{1, \ldots, k\}$, then the modified flip sequence

$$\alpha' := (a_1, \ldots, a_{i-1}, p(x, y'), a_{i+1} + \lambda(\tau), \ldots, a_k + \lambda(\tau)) \tag{38a}$$

produces a periodic path $P' = (x'_1, \ldots, x'_k)$ that visits necklaces in the same order as P, i.e., we have $\langle x_i\rangle = \langle x'_i\rangle$ for all $i = 1, \ldots, k$, and we have

$$\lambda(\alpha') = \lambda(\alpha) + \lambda(\tau). \tag{38b}$$

The situation where $(x_i, x_{i+1}) = (x, y')$ is symmetric, and can be analyzed with these equations by considering the inverted switch τ^{-1} with $\lambda(\tau^{-1}) = -\lambda(\tau)$.

Similarly, if we have $(x_i, x_{i+1}) = (y', x)$ for some $i \in \{1, \ldots, k\}$, then the modified flip sequence

$$\alpha' := (a_1, \ldots, a_{i-1}, p(x, y) + \lambda(\tau), a_{i+1} + \lambda(\tau), \ldots, a_k + \lambda(\tau)) \tag{38c}$$

produces a periodic path $P' = (x'_1, \ldots, x'_k)$ that visits necklaces in the same order as P, and we have

$$\lambda(\alpha') = \lambda(\alpha) + \lambda(\tau). \tag{38d}$$

Again, the situation where $(x_i, x_{i+1}) = (y, x)$ is symmetric, and can be analyzed with these equations by considering the inverted switch τ^{-1} with $\lambda(\tau^{-1}) = -\lambda(\tau)$.

In particular, if $\langle P\rangle$ is a Hamilton cycle in the necklace graph N_n, then $\langle P'\rangle$ is also a Hamilton cycle in the necklace graph, albeit one whose flip sequence has a different shift (as given by (38b) and (38d)).

For example, consider the flip sequence $\alpha = 6253462135$, which starting from $x_1 = 1110000$ produces the periodic path $P = (x_1, \ldots, x_{10})$ and the vertex x_{11} shown on the top left hand side of Figure 1 (recall that we omit the first bit here), and we have $\lambda(\alpha) = +1$. For the switch $\tau = (x, y, y') = 101\overline{0}\underline{0}10$ with $\lambda(\tau) = +5$ we have $(x_3, x_4) = (x, y)$, and according to (38a) the flip sequence $\alpha' = (6, 2, p(x, y'), 3+5, 4+5, 6+5, 2+5, 1+5, 3+5, 5+5) = 6241247613$ has shift $\lambda(\alpha') = \lambda(\alpha) + \lambda(\tau) = +1 + 5 = +6$ and produces a periodic path P' that visits necklaces in the same order as P. The path P' is shown on the top right hand side of Figure 1. All other columns with shifts $s = 2, 3, 4, 5$ in this figure were obtained from the first column by applying the same switching technique, using multiple different switches.

7.2. **Construction of switches.** We now describe a systematic way to construct many distinct switches from the canonic switch $\tau = 1^n\overline{0}0^{n-1}\underline{0}$, which has shift $\lambda(\tau) = +1$.

For any integers $n \geq 1$, $d \geq 1$ and $1 \leq s \leq d$, the (s, d)-*orbit* is the maximal prefix of the sequence $s + id$, $i \geq 0$, considered modulo $2n + 1$, in which all numbers are distinct. Clearly, the number of distinct (s, d)-orbits for fixed d and $s \geq 1$ is $n_d := \gcd(2n + 1, d)$, and the length of each orbit is $\ell_d := (2n+1)/\gcd(2n+1,d)$. Note that both n_d and ℓ_d are odd integers. For example, for $n=10$ and $d=6$ there are $n_d=3$ orbits of length $\ell_d=7$, namely the $(1,6)$-orbit $(1,7,13,19,4,10,16)$, the $(2,6)$-orbit $(2,8,14,20,5,11,17)$, and the $(3,6)$-orbit $(3,9,15,21,6,12,18)$. For any $n\geq 1$, we let X_n denote the set of all binary strings of length $2n$ with exactly n many 0s and n many 1s. For instance, we have $X_2=\{1100,1010,1001,0110,0101,0011\}$.

The base case of our definition is the switch $\tau_{n,1} := 1^n\overline{0}0^{n-1}\underline{0}$, which has shift $\lambda(\tau_{n,1})=+1$. For any integer $2\leq d\leq n$ that is coprime to $2n+1$, we let $\tau_{n,d}$ denote the sequence whose entries at the positions given by the $(1,d)$-orbit equal the sequence $\tau_{n,1}$, including the underlined and overlined bit. In words, $\tau_{n,d}$ is obtained by filling the entries of $\tau_{n,1}$ one by one into every dth position of $\tau_{n,d}$, starting at the first one.

For any integer $3\leq d\leq n$ that is not coprime to $2n+1$, we choose an arbitrary bitstring $x=(x_2,\ldots,x_{n_d})\in X_{(n_d-1)/2}$, and we let $\tau_{n,d,x}$ denote the sequence whose entries at the positions given by the $(1,d)$-orbit equal the sequence $\tau_{(\ell_d-1)/2,1}$, including the underlined and overlined bit, and for $j=2,\ldots,n_d$, all entries at the positions given by the (j,d)-orbit equal x_j. In words, $\tau_{n,d}$ is obtained by filling the entries of $\tau_{(\ell_d-1)/2,1}$ one by one into every dth position of $\tau_{n,d}$, starting from the first one, and then filling the gaps between these entries by copies of x. Clearly, the number of choices we have for x in this construction is $\binom{n_d-1}{(n_d-1)/2}$.

Note that the construction for coprime d can be understood as a special of the construction for non-coprime d with $n_d=1$ and $x=\varepsilon$.

These definitions are illustrated in Figure 19 for $n=1,\ldots,7$. The next lemma follows immediately from these definitions. It asserts that the sequences $\tau_{n,d}$ and $\tau_{n,d,x}$ defined before are indeed switches with shift d.

Lemma 18. *Let $n\geq 1$. For any integer $1\leq d\leq n$ that is coprime to $2n+1$, the sequence $\tau_{n,d}$ defined before is a switch with $\lambda(\tau_{n,d})=d$. For any integer $3\leq d\leq n$ that is not coprime to $2n+1$ and any bitstring $x\in X_{(n_d-1)/2}$, the sequence $\tau_{n,d,x}$ defined before is a switch with $\lambda(\tau_{n,d,x})=d$.*

In fact, every possible switch can be obtained in one of the two ways described by the lemma, and by reversal and cyclic rotations, but this is irrelevant here.

7.3. **Proof of Theorem 1 for $n\leq 38$.** Recall the definition of the function f from (4). We say that a switch $\tau=(x,y,y')$ is *f-conformal*, if $y=f(x)$ or if $x=f(y')$, and then we refer to (x,y) or (y',x), respectively, as the *f-edge* of the switch. Also, we say that τ is *f^{-1}-conformal*, if the inverted switch τ^{-1} is f-conformal, and we refer to the f-edge of τ^{-1} also as the f-edge of τ. A switch being f-conformal means that its f-edge belongs to a periodic path defined in (8a).

Given a set of nesting-free gluing pairs $G\subseteq G_n$, we say that an f-conformal or f^{-1}-conformal switch τ is *usable w.r.t. G*, if for every gluing pair $(\hat{x},\hat{y})\in G$ and all $i\geq 0$, the three f-edges of the gluing cycle $\sigma^i(C(\hat{x},\hat{y}))$ defined in (12), i.e., the edges $\sigma^i((\hat{x}^0,\hat{x}^1))$, $\sigma^i((\hat{x}^5,\hat{x}^6))$ and $\sigma^i((\hat{y}^0,\hat{y}^1))$ as defined in (10) are distinct from the f-edges of τ. Recall from (14) and (19) that the three f-edges are *removed* when joining periodic paths, so a switch whose f-edge is one of the removed edges would not be relevant for us. We also say that a usable switch τ is *reversed*, if the f-edge of τ lies on the reversed path of one of the gluing cycles $\sigma^i(C(\hat{x},\hat{y}))$, $(\hat{x},\hat{y})\in G$, for some $i\geq 0$, i.e., on the path $\sigma^i((\hat{x}^1,\ldots,\hat{x}^5))$.

For an f-conformal usable switch τ that is not reversed, the modifications to the flip sequence described by (38) change the shift by $+\lambda(\tau)$, and for an f^{-1}-conformal usable switch that is not reversed, they change the shift by $+\lambda(\tau^{-1})=-\lambda(\tau)$. On the other hand, if the switch is reversed, then the sign of these changes is inverted. We refer to this quantity as the *effective shift* of τ, and we denote it by $\lambda^e(\tau)$; see Figure 19. Essentially, the effective shift of τ is the shift $\lambda(\tau)$ with the bit flipped by f

bit flipped by f^{-1}

conformal: $\bar{0}\,\underline{0} \to -$; $\underline{0}\,\bar{0} \to +$

		$d=\lambda$	conformal	usable	reversed	eff. shift λ^e
$n=1$	$1\,\bar{0}\,\underline{0}$	1	$-$			
$n=2$	$1\,1\,\bar{0}\,0\,\underline{0}$	1	$-$			
	$1\,0\,1\,\underline{0}\,\bar{0}$	2	$+$			
$n=3$	$1\,1\,1\,\bar{0}\,0\,0\,\underline{0}$	1	$-$			
	$1\,0\,1\,0\,1\,\underline{0}\,\bar{0}$	2	$+$			
	$1\,0\,\bar{0}\,1\,\underline{0}\,0\,1$	3	$-$			
$n=4$	$1\,1\,1\,1\,\bar{0}\,0\,0\,0\,\underline{0}$	1	$-$	y	y	$+1$
	$1\,0\,1\,0\,1\,0\,1\,\underline{0}\,\bar{0}$	2	$+$	y	n	$+2$
	$1\,1\,0\,\bar{0}\,1\,0\,\underline{0}\,1\,0$	3	$-$	y	n	-3
	$1\,0\,1\,\bar{0}\,0\,1\,\underline{0}\,0\,1$	3	n			
	$1\,0\,0\,1\,1\,\underline{0}\,0\,\bar{0}\,1$	4	$+$	y	n	$+4$
$n=5$	$1\,1\,1\,1\,1\,\bar{0}\,0\,0\,0\,0\,\underline{0}$	1	$-$	y	y	$+1$
	$1\,0\,1\,0\,1\,0\,1\,0\,1\,\underline{0}\,\bar{0}$	2	$+$	y	n	$+2$
	$1\,1\,0\,1\,\bar{0}\,0\,1\,0\,\underline{0}\,1\,0$	3	$-$	y	n	-3
	$1\,1\,0\,0\,1\,1\,0\,\underline{0}\,1\,\bar{0}\,0$	4	n			
	$1\,0\,0\,\bar{0}\,1\,1\,\underline{0}\,0\,0\,1\,1$	5	$-$	y	n	-5
$n=6$	$1\,1\,1\,1\,1\,1\,\bar{0}\,0\,0\,0\,0\,0\,\underline{0}$	1	$-$	y	y	$+1$
	$1\,0\,1\,0\,1\,0\,1\,0\,1\,0\,1\,\underline{0}\,\bar{0}$	2	$+$	y	n	$+2$
	$1\,0\,1\,1\,0\,\bar{0}\,1\,0\,0\,1\,\underline{0}\,0\,1$	3	n			
	$1\,0\,0\,1\,1\,0\,0\,1\,1\,\underline{0}\,0\,\bar{0}\,1$	4	$+$	y	n	$+4$
	$1\,0\,1\,0\,\bar{0}\,1\,0\,1\,\underline{0}\,0\,1\,0\,1$	5	n			
	$1\,0\,0\,0\,1\,1\,1\,\underline{0}\,0\,0\,\bar{0}\,1\,1$	6	$+$	y	n	$+6$
$n=7$	$1\,1\,1\,1\,1\,1\,1\,\bar{0}\,0\,0\,0\,0\,0\,0\,\underline{0}$	1	$-$	y	y	$+1$
	$1\,0\,1\,0\,1\,0\,1\,0\,1\,0\,1\,0\,1\,\underline{0}\,\bar{0}$	2	$+$	y	n	$+2$
	$1\,1\,0\,1\,1\,0\,\bar{0}\,1\,0\,0\,1\,0\,\underline{0}\,1\,0$	3	$-$	y	n	-3
	$1\,0\,1\,1\,0\,1\,\bar{0}\,0\,1\,0\,0\,1\,\underline{0}\,0\,1$	3	n			
	$1\,1\,0\,0\,1\,1\,0\,0\,1\,1\,0\,\underline{0}\,1\,\bar{0}\,0$	4	n			
	$1\,1\,1\,0\,0\,\bar{0}\,1\,1\,0\,0\,\underline{0}\,1\,1\,0\,0$	5	$-$	y	n	-5
	$1\,1\,0\,1\,0\,\bar{0}\,1\,0\,1\,0\,\underline{0}\,1\,0\,1\,0$	5	$-$	y	n	-5
	$1\,1\,0\,0\,1\,\bar{0}\,1\,0\,0\,1\,\underline{0}\,1\,0\,0\,1$	5	n			
	$1\,0\,1\,1\,0\,\bar{0}\,0\,1\,1\,0\,\underline{0}\,0\,1\,1\,0$	5	n			
	$1\,0\,1\,0\,1\,\bar{0}\,0\,1\,0\,1\,\underline{0}\,0\,1\,0\,1$	5	n			
	$1\,0\,0\,1\,1\,\bar{0}\,0\,0\,1\,1\,\underline{0}\,0\,0\,1\,1$	5	n			
	$1\,1\,0\,0\,1\,0\,1\,1\,0\,\underline{0}\,1\,0\,\bar{0}\,1\,0$	6	$+$	y	n	$+6$
	$1\,0\,1\,0\,0\,1\,1\,0\,1\,\underline{0}\,0\,1\,\bar{0}\,0\,1$	6	n			
	$1\,0\,0\,0\,\bar{0}\,1\,1\,1\,\underline{0}\,0\,0\,0\,1\,1\,1$	7	$-$	y	n	-7

FIGURE 19. All switches for $n = 1, \ldots, 7$. The switch $\tau_{n,1}$ is shown as the first switch in each block, and the remaining switches are ordered by increasing d. The bits flipped by f and f^{-1} are marked light gray and dark gray, respectively. The framed bits belong to a $(1,d)$-orbit for some d that is not coprime to $2n+1$. Whether a switch is f-conformal or f^{-1}-conformal is indicated by $+$ or $-$, respectively, and by 'n' if neither of the two. Similarly, a switch being usable or reversed is indicated by 'y'=yes and 'n'=no. The resulting effective shifts are shown in the rightmost column.

sign determined by f-conformality (multiplied by -1 iff f^{-1}-conformal) and reversed (multiplied by -1 iff reversed). The effective shift describes by how much the shift of the flip sequence along a periodic path changes when applying the aforementioned switching technique using this switch.

To check whether τ is usable, we consider its f-edge, and we distinguish two cases: If the f-edge of τ is (x,y) with $x \in A_n$ and $y \in B_n$, then we only need to check that $(x,y) \notin \{\sigma^i((\hat{x}^0,\hat{x}^1)), \sigma^i((\hat{y}^0,\hat{y}^1)) \mid (\hat{x},\hat{y}) \in G \wedge i \geq 0\}$. Recall from (10) that $\hat{x}^0 = 1\,1\,0\,u\,0\,v\,0$ and $\hat{y}^0 = 1\,0\,1\,u\,0\,v\,0$ for some $u,v \in D$, so if $x' := \sigma^{\ell(x)}(x)$ with $\ell(x)$ as in Lemma 5 satisfies

$$x' = 1\,1\,1\cdots, \tag{i}$$

i.e., the first three bits of x' are 1s (the first bit is always 1), then τ is usable for *every* G. On the other hand, if the f-edge of τ is (y',x) with $y' \in B_n$ and $x \in A_n$, we only need to check that $(y',x) \notin \{\sigma^i((\hat{x}^5,\hat{x}^6)) \mid (\hat{x},\hat{y}) \in G \wedge i \geq 0\}$. Recall from (10) that $\hat{x}^6 = 1\,0\,0\,u\,1\,v\,0$ for some $u,v \in D$, and therefore $\sigma^{\ell(\hat{x}^6)}(\hat{x}^6) = \sigma^3(\hat{x}^6) = u\,1\,v\,0\,1\,0\,0$, so if $x' := \sigma^{\ell(x)}(x)$ satisfies

$$x' = \cdots 0\,0\,0, \tag{ii}$$

i.e., the last three bits of x' are 0s (the last two bits are always 0s), then τ is usable for *every* G. On the other hand, if $x' = \cdots 1\,0\,0$, then we may consider the last five bits of x', and if

$$x' = \cdots 1\,0\,1\,0\,0, \tag{iii}$$

then this implies that the substring v of $\hat{x}^6$ satisfies $v = \varepsilon$, i.e., the right subtree of $\hat{x}$ and $\hat{y}$ in the gluing pair $(\hat{x}, \hat{y})$ is empty. This is in principle possible for arbitrary sets of gluing pairs G, but not for the ones arising from our spanning tree $\mathcal{T}_n \subseteq \mathcal{H}_n$ defined in Section 6.1. Specifically, if $G = G(\mathcal{T}_n)$, then recall from the proof of Lemma 17 that for all gluing pairs $(\hat{x}, \hat{y}) \in G(\mathcal{T}_n)$, the root of $\hat{x}$ is not a leaf, i.e., for such an $\hat{x} = 1\,u\,0\,v$ with $u, v \in D$, we have $v \neq \varepsilon$. We can thus conclude from (iii) that τ is usable w.r.t. $G = G(\mathcal{T}_n)$. If none of the sufficient conditions (i)–(iii) applies, we can still check whether τ is usable by considering the definition of $\mathcal{T}_n$ in more detail.

To check whether τ is reversed, we consider its f-edge (x, y) with $x \in A_n$ and $y \in B_n$, or its f-edge (y', x) with $y' \in B_n$ and $x \in A_n$, and if both rooted trees $x' := \rho^{-1}(t(x)) \in D_n$ and $x'' := \rho^{-2}(x)(t(x)) \in D_n$ (recall Proposition 7 (i)) do not have the form (9) or have a root that is a leaf, i.e., we have

$$\begin{aligned} x' \in \{1\,0\,\cdots, 1\,1\,1\,\cdots\} &\text{ or the root of } x' \text{ is a leaf,} \\ \text{and } x'' \in \{1\,0\,\cdots, 1\,1\,1\,\cdots\} &\text{ or the root of } x'' \text{ is a leaf,} \end{aligned} \tag{39}$$

then the switch is *not* reversed. If this sufficient condition does not apply, checking whether a switch is reversed or not requires considering the definition of $\mathcal{T}_n$ in more detail.

Proof of Theorem 1 *for* $n \leq 38$. For $n = 1$ we can use the flip sequence $\alpha_0 := 21$ for $s = 1$ and $\alpha_0 := 31$ for $s = 2$, starting from $x_1 := 1100$. For $n = 2$ we can use $\alpha_0 := 5135$ for $s = 1$, $\alpha_0 := 3241$ for $s = 2$, $\alpha_0 := 5142$ for $s = 3$, and $\alpha_0 := 3253$ for $s = 4$, starting from $x_1 := 111000$. For $n = 3$ and $1 \leq s \leq 2n = 6$ valid solutions are given in Figure 1.

For the rest of the proof we assume that $n \geq 4$. We consider the spanning tree $\mathcal{T}_n \subseteq \mathcal{H}_n$ defined in Section 6.1. As explained in Section 5.6, based on the spanning tree $\mathcal{T}_n$, we define a periodic path P with starting vertex $x_1 := 1^n 0^{n+1}$ and second vertex $f(x_1)$ in the middle levels graph M_n, such that $\langle P \rangle$ is a Hamilton cycle in the necklace graph N_n, and the shift of the corresponding flip sequence $\alpha(P)$ is given by (23). As the spanning tree $\mathcal{T}_n$ is nesting-free by Lemma 17, all signs $\gamma_T \in \{-1, +1\}$ in this sum are positive, and we therefore have $\lambda(\alpha(P)) = C_n$ by (36), with C_n being the nth Catalan number.

We modify the flip sequence $\alpha(P)$ as described by (38) by a set S of f-conformal or f^{-1}-conformal switches that are usable w.r.t. to the nesting-free set of gluing pairs $G = G(\mathcal{T}_n)$. This yields a path P' that visits necklaces in the same order as P, and the corresponding flip sequence $\alpha'(S)$ has shift

$$\lambda(\alpha'(S)) = C_n + \sum_{\tau \in S} \lambda^{\mathrm{e}}(\tau), \tag{40}$$

where $\lambda^{\mathrm{e}}(\tau)$ is the effective shift of τ. We aim to choose S so that this sum has any possible value s that is coprime to $2n + 1$. For this it is enough to choose S so that modulo $2n + 1$, any possible value in $\{0, \ldots, 2n\}$ can be achieved.

To this end, we say that a multiset S of integers is *m-complete* if modulo m every possible number in $\{0, \ldots, m - 1\}$ arises as a sum of a subset of S. For example, the multiset $\{-1, +2, -3, +5, +5\}$ is 17-complete, as for $S_0 := \emptyset$, $S_1 := \{-1, +2\}$, $S_2 := \{+2\}$, $S_3 := \{-1, +2, -3, +5\}$, $S_4 := \{-1, +5\}$, $S_5 := \{+5\}, \ldots, S_{14} := \{-3\}$, $S_{15} := \{-1, +2, -3\}$, $S_{16} := \{-1\}$ we have $\sum_{x \in S_i} = i$ modulo 17 for all $i = 0, \ldots, 16$.

Appendix A shows for every $4 \leq n \leq 38$ a set S' of f-conformal or f^{-1}-conformal switches (each row in the tables contains one switch), all of which were constructed via Lemma 18. All of these switches and their cyclic rotations are usable w.r.t. $G = G(\mathcal{T}_n)$, and the conditions (i)–(iii) that apply to obtain this are listed in the last column of these tables. In the four exceptional cases marked by (iv1)–(iv4), none of these conditions applies. However, the gluing pair $(\hat{x}, \hat{y}) \in G_n$ for which an f-edge of the gluing cycle $\sigma^i(C(\hat{x}, \hat{y}))$ for some $i \geq 0$ coincides with the f-edge of this switch is still *not* in the set $G(\mathcal{T}_n)$, which can be checked by straightforward calculations, using the definition of $\mathcal{T}_n$ and considering the left and right subtrees $u, v \in D$ of $\hat{x}$, which are as follows in these four cases:

$$(u, v) = (10, 10), \tag{iv1}$$

$$(u, v) = (10, 1010), \tag{iv2}$$

$$(u, v) = (10, 1011011010010010), \tag{iv3}$$

$$(u, v) = (1011011010010010, 1011010010). \tag{iv4}$$

The first switch in each of the tables in the appendix is reversed (marked with 'R' in the last column), as its f-edge lies on the reversed path of the gluing cycle $\sigma^2(C(\hat{x}, \hat{y}))$ for $(\hat{x}, \hat{y}) := (11001^{n-2}0^{n-2}, \mathrm{pull}(\hat{x}))$ and we have $(\hat{x}, \hat{y}) \in G(\mathcal{T}_n)$ by the definition of $\mathcal{T}_n$. No other switch in the tables is reversed, which can be verified in each case by applying condition (39). The resulting effective shift for each switch is listed in the second-to-last column of the tables. Moreover, the corresponding multisets of integers $\{\lambda^e(\tau) \mid \tau \in S'\}$ can easily be checked to be $(2n+1)$-complete.

It follows that for each of these values of n and for any $1 \leq s \leq 2n$ that is coprime to $2n + 1$, there is a subset $S \subseteq S'$ such that the flip sequence $\alpha'(S)$ obtained by applying a suitable cyclic rotation of each switch $\tau \in S$ has a shift of $\lambda(\alpha'(S)) = s$ by (40). We may then define $\alpha_0 := \alpha'(S)$, and the remaining α_i for $i = 1, \ldots, 2n$ as in (24), and from there we complete the proof as explained in Section 5.6. □

7.4. **Discussion of the switching technique.** To control the shift value of flip sequences, the switching technique described before is undoubtedly much more elegant than the spanning tree modification described in Section 5.7. It also yields much nicer Gray codes, as the order of necklaces remains unchanged under switching. Unfortunately, despite considerable efforts, we failed to make the switching technique work for general values of n. In particular, it is not even known what the value of the nth Catalan number modulo $(2n + 1)$ is; recall (40). For $n \geq 2$ and $2n + 1$ being prime, this value is $+2$ or -2, as can be shown easily, but things are much more complicated for non-prime values $2n + 1$. The first few entries of this sequence are $1, 2, -2, -4, -2, 2, -6, 2, -2, -4, -2, 12, -5, 2, -2, \ldots = 1, 2, 5, 5, 9, 2, 9, 2, 17, 17, 21, 12, 22, 2, 29, \ldots$. While Lemma 18 is a very powerful tool to provide us with many distinct switches (in fact, all possible switches), we have unfortunately little control over which of them are f-conformal or f^{-1}-conformal. The proof of Theorem 1 for small n and several computer experiments that we performed suggest that there are enough conformal and usable switches available for all n, but we are unable to prove this. We can systematically construct conformal switches that yield $(2n + 1)$-complete sets of effective shift values only in the following two cases: n being a power of 2, or $2n + 1$ having two large factors. We failed to do so in general, in particular in the case when $2n + 1$ is prime. It is not even clear which multisets of integers one should aim for to obtain a $(2n + 1)$-complete set, which is an interesting purely number-theoretic problem. While some general sufficient criteria in this direction are known (see e.g. [HLS08]), none of them seem to be applicable in our situation. Overall, it remains open whether the switching technique can be used for every n, which would simplify our proofs.

8. Proof of Theorem 2

Our algorithm to compute a star transposition ordering of $(n+1, n+1)$-combinations is a faithful implementation of the constructive proof of Theorem 1 presented in Section 5.8 for $n \geq 39$ and in Section 7.3 for $n \leq 38$. For the reasons discussed at the beginning of Section 6, in both cases we use the spanning tree $\mathcal{T}_n$ of $\mathcal{H}_n$ defined in Section 6.1. This is possible, as the proof of Theorem 1 for $n \geq 39$ works also with this redefined spanning tree $\mathcal{T}_n$. In particular, Proposition 15 (iv) also holds for this spanning tree $\mathcal{T}_n$. To see this, in addition to the leaves of all plane trees in L_β that are pushable from the centroid, we now also have to consider all leaves that are pullable from the centroid (marked by black squares in Figure 13), and that yield a plane tree not in L_β. However, this gives exactly the plane trees T_β^1, T_β^2, $\widetilde{T}_\beta^2$, and T_β^3. As each of these trees has a unique arm with 7 edges that is considered with highest priority by rule (i) in step (T2), these trees are not connected to a tree in L_β in $\mathcal{T}_n$.

Proof of Theorem 2. In the following we outline the key data structures and computation steps performed by our algorithm. For more details, see the C++ implementation available at [cos]. We maintain the following data structures:

- the bitstring representation $x \in A_n \cup B_n$ of the current $(n+1, n+1)$-combination;
- the position $\ell(x)$ from where to read the rooted tree $t(x)$ in x;
- the plane tree $T = [t(x)]$ and its centroid(s).

The space required by these data structures is clearly $\mathcal{O}(n)$.

There are two types of steps that we encounter in our algorithm: An *f-step* is simply an application of the mapping f defined in (4) to the current bitstring x, which corresponds to following one of the basic flip sequences. Such a step incurs only a rotation of the tree $t(x)$ (recall (5)), and therefore the plane tree $T = [t(x)] = [\rho(t(x))]$ is not modified. On a subpath that is reversed by a gluing cycle, we apply f^{-1} and inverse tree rotation $\rho^{-1}(t(x))$ instead. A *pull/push step* is more complicated, and corresponds to following one of the edges of a gluing cycles $\sigma^i(C(\hat{x}, \hat{y}))$, $i \geq 0$, $(\hat{x}, \hat{y}) \in G(\mathcal{T}_n)$ for some arc $([\hat{x}], [\hat{y}])$ in the spanning tree $\mathcal{T}_n$. Such a step also modifies the plane tree $T = [t(x)]$ by applying a pull or push operation to one of its leaves. All these updates can easily be done in time $\mathcal{O}(n)$.

For deciding whether to perform an f-step or a pull/push step, the following computations are performed on the current plane tree $T = [t(x)]$, following the steps (T1)–(T3) described in Section 6.1:

- compute a centroid c of T and its potential $\varphi(c)$ as in step (T1) in time $\mathcal{O}(n)$ (see [KA76]);
- compute the lexicographic subtree ordering as in step (T1) in time $\mathcal{O}(n)$. In the case where the centroid is unique, this is achieved by Booth's algorithm [Boo80]. Specifically, to compute the lexicographically smallest ccw ordering $(t_1, \ldots, t_k)$ of the c-subtrees of T we insert -1s as separators between the bitstring representations $t_1, \ldots, t_k$ of the subtrees, i.e., we consider the string $z := (-1, t_1, -1, \ldots, -1, t_k)$. This trick makes Booth's algorithm return a cyclic rotation of z that starts with -1, and it is easy to check that this rotation is also the one that minimizes the cyclic subtree ordering $(t_1, \ldots, t_k)$.
- compute a c-subtree of T and one of its leaves as in steps (T2) and (T3) in Section 6.1 in time $\mathcal{O}(n)$.

Overall, the decision which type of step to perform next takes time $\mathcal{O}(n)$ to compute.

Upon initialization, the algorithm once computes the value of the nth Catalan number C_n modulo $2n+1$ in time $\mathcal{O}(n^2)$, using Segner's recurrence relation. For $n \leq 38$ we proceed as follows: With the shift s specified as input to the algorithm, we compute $r \in \{0, \ldots, 2n\}$ such that $C_n + r = s$ modulo $2n+1$, and we consider a precomputed set of switches $S \subseteq S'$ with S' as specified in the tables in the appendix such that $\sum_{\tau\in S} \lambda^e(\tau) = r$. Whenever we encounter a switch in the course of the algorithm, which can be detected in time $\mathcal{O}(n)$, we perform a modified flip as described by (38). Each time this happens, the position $\ell(x)$ has to be recomputed, while the plane tree $T = [t(x)]$ does not change.

On the other hand, for $n \geq 39$ we proceed as follows: With the shift s specified as input, we compute $r \in \{0, \ldots, 2n\}$ such that $C_n + 2 \cdot r = s$ modulo $2n+1$. We then use the spanning tree $\mathcal{T}_n(\chi)$ defined in (34) for the sign sequence χ whose first r entries are equal to $-$, and all others are equal to $+$. Recall that χ has length 2^k with k as defined in (27), and $2^k \geq 2n \geq r$ by the assumption $n \geq 39$. As $\mathcal{T}_n$ is nesting-free by Lemma 17, we have $\gamma_T = +1$ for all $T \in T_n$ in (35), except for the tree $L^0_\beta \in L_\beta$ for each β with $\chi_\beta = -$, which satisfies $\lambda(L^0_\beta) = 2n$ by Proposition 15 (ii). Consequently, the shift of the corresponding flip sequence evaluates to $\lambda(\alpha(P(\chi))) = \sum_{T\in T_n} \lambda(T) - 4n \cdot r$, which equals $C_n + 2 \cdot r$ by (36) and the fact that $-4n = +2$ modulo $2n+1$, and this is equal to s by the definition of r. Working with $\mathcal{T}_n(\chi)$ instead of $\mathcal{T}_n$ requires bypassing the aforementioned decision routine in the cases where the current plane tree $T = [t(x)]$ belongs to one of the sets $L_\beta \cup \{T^5_\beta\}$ defined in (32), which can easily be detected in time $\mathcal{O}(n)$.

Summarizing, the algorithm described before runs in time $\mathcal{O}(n)$ in each step, using $\mathcal{O}(n)$ memory in total, and it requires time $\mathcal{O}(n^2)$ for initialization. □

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Appendix A. Usable switches for $n \leq 38$

The following tables show the sets S' of switches used in the proof of Theorem 1 for $n \leq 38$.

$n = 4$	λ^e	usable
111100000	+1	(ii) R
101010100	+2	(iii)
110010010	−3	(iv1)
100110001	+4	(ii)

$n = 5$	λ^e	usable
11111000000	+1	(ii) R
10101010100	+2	(iii)
11010010010	−3	(iv2)
10001100011	−5	(i)

$n = 6$	λ^e	usable
1111110000000	+1	(ii) R
1010101010100	+2	(iii)
1001100110001	+4	(ii)
1000111000011	+6	(ii)

$n = 7$	λ^e	usable
111111100000000	+1	(ii) R
101010101010100	+2	(iii)
111000110001100	−5	(ii)
110100101001010	−5	(iii)
100001110000111	−7	(i)

$n = 8$	λ^e	usable
11111111000000000	+1	(ii) R
10101010101010100	+2	(iii)
10011001100110001	+4	(ii)
11010100101001010	−5	(iii)
10000111100000111	+8	(ii)

$n = 9$	λ^e	usable
1111111110000000000	+1	(ii) R
1010101010101010100	+2	(iii)
1110011000110001100	−5	(ii)
1000111000111000011	+6	(ii)
1000001111000001111	−9	(i)

$n = 10$	λ^e	usable
111111111100000000000	+1	(ii) R
101010101010101010100	+2	(iii)
100110011001100110001	+4	(ii)
111100001110000111000	−7	(ii)
111010001101000110100	−7	(ii)

$n = 11$	λ^e	usable
11111111111000000000000	+1	(ii) R
10101010101010101010100	+2	(iii)
11011011010010010010010	−3	(iv3)
11010101001010100101010	−7	(iii)
10000001111100000011111	−11	(i)

$n = 12$	λ^e	usable
1111111111110000000000000	+1	(ii) R
1010101010101010101010100	+2	(iii)
1001100110011001100110001	+4	(ii)
1110011100011000110001100	−5	(ii)
1101011010010100101001010	−5	(iii)
1000011110000111100000111	+8	(ii)

$n = 13$	λ^e	usable
111111111111100000000000000	+1	(ii) R
101010101010101010101010100	+2	(iii)
110101101010010100101001010	−5	(iii)
111100011100001110000111000	−7	(ii)
111110000011110000011110000	−9	(ii)
111101000011101000011101000	−9	(ii)

$n = 14$	λ^e	usable
11111111111111000000000000000	+1	(ii) R
10101010101010101010101010100	+2	(iii)
10011001100110011001100110001	+4	(ii)
11100111001100011000110001100	−5	(ii)
11010101010010101010010101010	−9	(iii)
10101001010110101001010010101	+12	(iii)

$n = 15$	λ^e	usable
1111111111111110000000000000000	+1	(ii) R
1010101010101010101010101010100	+2	(iii)
1000111000111000111000111000011	+6	(ii)
1110011001100011001100011001100	−9	(ii)
1000001111100000111110000001111	+10	(ii)
1010010010110110100100100101101	+14	(iv4)

$n = 16$	λ^e	usable
111111111111111100000000000000000	+1	(ii) R
101010101010101010101010101010100	+2	(iii)
100110011001100110011001100110001	+4	(ii)
100001111000011110000111100000111	+8	(ii)
111111000000111110000001111100000	−11	(ii)
111110100000111101000001111010000	−11	(ii)

$n = 17$	λ^e	usable
11111111111111111000000000000000000	+1	(ii) R
10101010101010101010101010101010100	+2	(iii)
11100111001110001100011000110001100	−5	(ii)
11010110101101001010010100101001010	−5	(iii)
11110001111000011100001110000111000	−7	(ii)
11100011001110001100111000110001100	+10	(ii)
11010010101101001010110100101001010	+10	(iii)

$n = 18$	λ^e	usable
1111111111111111110000000000000000000	+1	(ii) R
1010101010101010101010101010101010100	+2	(iii)
1001100110011001100110011001100110001	+4	(ii)
1101011010110101001010010100101001010	−5	(iii)
1000111000111000111000111000111000011	+6	(ii)
1101010110101010010101001010100101010	−7	(iii)
1000000111111000000111111000000011111	+12	(ii)

$n = 19$	λ^e	usable
111111111111111111100000000000000000000	+1	(ii) R
101010101010101010101010101010101010100	+2	(iii)
111111100000001111110000000111111000000	−13	(ii)
111111010000001111101000000111110100000	−13	(ii)
101010100101010110101010010101001010101	+16	(iii)
100000000001111111110000000000111111111	−19	(i)

$n = 20$	λ^e	usable
11111111111111111111000000000000000000000	+1	(ii) R
10101010101010101010101010101010101010100	+2	(iii)
10011001100110011001100110011001100110001	+4	(ii)
11110001111000111000011100001110000111000	−7	(ii)
10000111100001111000011110000111100000111	+8	(ii)
10000011111000001111100000111110000001111	+10	(ii)
10101001010110101001010110101001010010101	+12	(iii)

$n = 21$	λ^e	usable
1111111111111111111110000000000000000000000	+1	(ii) R
1010101010101010101010101010101010101010100	+2	(iii)
1000111000111000111000111000111000111000011	+6	(ii)
1111110000011111000000111110000001111100000	−11	(ii)
1110011001100110001100110011000110011001100	−13	(ii)
1000000000001111111111000000000001111111111	−21	(i)

$n = 22$	λ^e	usable
111111111111111111111100000000000000000000000	+1	(ii) R
101010101010101010101010101010101010101010100	+2	(iii)
100110011001100110011001100110011001100110001	+4	(ii)
111001110011100111000110001100011000110001100	−5	(ii)
111110000111110000011110000011110000011110000	−9	(ii)
111000110011100011001110001100111000110001100	+10	(ii)
111100011100011100001110001110000111000111000	−13	(ii)

$n = 23$	λ^e	usable
11111111111111111111111000000000000000000000000	+1	(ii) R
10101010101010101010101010101010101010101010100	+2	(iii)
11010110101101011010100101001010010100101001010	−5	(iii)
11010101011010101010010101010010101010010101010	−9	(iii)
10011000110011100110001100111001100011000110011	+14	(ii)
11010101010101010010101010101010010101010101010	−15	(iii)
10000000000001111111111100000000000011111111111	−23	(i)

$n = 24$	λ^e	usable
1111111111111111111111110000000000000000000000000	+1	(ii) R
1010101010101010101010101010101010101010101010100	+2	(iii)
1001100110011001100110011001100110011001100110001	+4	(ii)
1000111000111000111000111000111000111000111000011	+6	(ii)
1111000111100011110000111000011100001110000111000	−7	(ii)
1110100111010011101000110100011010001101000110100	−7	(ii)
1101010110101011010100101010010101001010100101010	−7	(iii)
1111000011100011110000111000111100001110000111000	+14	(ii)

$n = 25$	λ^e	usable
111111111111111111111111100000000000000000000000000	+1	(ii) R
101010101010101010101010101010101010101010101010100	+2	(iii)
110101011010101101010100101010010101001010100101010	−7	(iii)
100000111110000011111000001111100000111110000001111	+10	(ii)
111111100000011111100000001111110000000111111000000	−13	(ii)
111111111000000000111111110000000001111111100000000	−17	(ii)
111111101000000000111111101000000001111111010000000	−17	(ii)

$n = 26$	λ^e	usable
11111111111111111111111111000000000000000000000000000	+1	(ii) R
10101010101010101010101010101010101010101010101010100	+2	(iii)
10011001100110011001100110011001100110011001100110001	+4	(ii)
11111000011111000011110000011110000011110000011110000	−9	(ii)
10101001010110101001010110101001010110101001010010101	+12	(iii)
11010101010101010100101010101010101001010101010101010	−17	(iii)
10011001100011001100111001100110001100110001100110011	+22	(ii)

$n = 27$	λ^e	usable
1111111111111111111111111110000000000000000000000000000	+1	(ii) R
1010101010101010101010101010101010101010101010101010100	+2	(iii)
1110011100111001110011100011000110001100011000110001100	−5	(ii)
1101011010110101101011010010100101001010010100101001010	−5	(iii)
1000111000111000111000111000111000111000111000111000011	+6	(ii)
1110001100111000110011100011001110001100111000110001100	+10	(ii)
1110011100011001110001100011001110001100011001110001100	−15	(ii)
1101011010010101101001010010101101001010010101101001010	−15	(iii)

$n = 28$	λ^e	usable
111111111111111111111111111100000000000000000000000000000	+1	(ii) R
101010101010101010101010101010101010101010101010101010100	+2	(iii)
100110011001100110011001100110011001100110011001100110001	+4	(ii)
110101101011010110101101010010100101001010010100101001010	−5	(iii)
110101010101101010101010010101010101001010101001010101010	−11	(iii)
100000001111111000000011111110000000111111100000000111111	+14	(ii)
111111111100000000001111111110000000000111111111000000000	−19	(ii)

$n = 29$	λ^e	usable
11111111111111111111111111111000000000000000000000000000000	+1	(ii) R
10101010101010101010101010101010101010101010101010101010100	+2	(iii)
11100111001110011100111001100011000110001100011000110001100	−5	(ii)
11111111000000011111110000000011111110000000011111110000000	−15	(ii)
11111000011110000111100000111100001111000001111000011110000	−17	(ii)
11010101010101010101001010101010101010100101010101010101010	−19	(iii)
10000000000000001111111111111100000000000000011111111111111	−29	(i)

$n = 30$	λ^e	usable
1111111111111111111111111111110000000000000000000000000000000	+1	(ii) R
1010101010101010101010101010101010101010101010101010101010100	+2	(iii)
1001100110011001100110011001100110011001100110011001100110001	+4	(ii)
1000111000111000111000111000111000111000111000111000111000011	+6	(ii)
1000001111100000111110000011111000001111100000111110000001111	+10	(ii)
1000000111111000000111111000000111111000000111111000000011111	+12	(ii)
1001100011001110011000110011100110001100111001100011000110011	+14	(ii)
1000000000011111111110000000000111111111100000000000111111111	+20	(ii)

$n = 31$	λ^e	usable
111111111111111111111111111111100000000000000000000000000000000	+1	(ii) R
101010101010101010101010101010101010101010101010101010101010100	+2	(iii)
111100011110001111000111100001110000111000011100001110000111000	−7	(ii)
111010011101001110100111010001101000110100011010001101000110100	−7	(ii)
110101011010101101010110101001010100101010010101001010100101010	−7	(iii)
111110000111110000111110000011110000011110000011110000011110000	−9	(ii)
111101000111101000111101000011101000011101000011101000011101000	−9	(ii)
111100100111100100111100100011100100011100100011100100011100100	−9	(ii)
111100001110001111000011100011110000111000111100001110000111000	+14	(ii)
111010001101001110100011010011101000110100111010001101000110100	+14	(ii)

$n = 32$	λ^e	usable
11111111111111111111111111111111000000000000000000000000000000000	+1	(ii) R
10101010101010101010101010101010101010101010101010101010101010100	+2	(iii)
10011001100110011001100110011001100110011001100110011001100110001	+4	(ii)
11100111001110011100111001110001100011000110001100011000110001100	−5	(ii)
11010110101101011010110101101001010010100101001010010100101001010	−5	(iii)
11100011001110001100111000110011100011001110001100111000110001100	+10	(ii)
11100011000110011100111000110001100111001110001100011000110011100	+20	(ii)
11010010100101011010110100101001010110101101001010010100101011010	+20	(iii)

$n = 33$	λ^e	usable
1111111111111111111111111111111110000000000000000000000000000000000	+1	(ii) R
1010101010101010101010101010101010101010101010101010101010101010100	+2	(iii)
1101011010110101101011010110101001010010100101001010010100101001010	−5	(iii)
1000111000111000111000111000111000111000111000111000111000111000011	+6	(ii)
1110011001110011001110011001100011001100011001100011001100011001100	−9	(ii)
1101010101010110101010101010010101010101001010101010100101010101010	−13	(iii)
1111111110000000011111111000000000111111110000000001111111100000000	−17	(ii)
1000111000011100011110001110000111000111100011100001110000111000111	+20	(ii)

$n = 34$	λ^e	usable
111111111111111111111111111111111100000000000000000000000000000000000	+1	(ii) R
101010101010101010101010101010101010101010101010101010101010101010100	+2	(iii)
100110011001100110011001100110011001100110011001100110011001100110001	+4	(ii)
111001110011100111001110011100110001100011000110001100011000110001100	−5	(ii)
111001100110011100110011001100011001100110001100110011000110011001100	−13	(ii)
101010101001010101011010101010010101010110101010100101010100101010101	+20	(iii)
111111111111000000000000111111111110000000000001111111111100000000000	−23	(ii)

$n = 35$	λ^e	usable
11111111111111111111111111111111111000000000000000000000000000000000000	+1	(ii) R
10101010101010101010101010101010101010101010101010101010101010101010100	+2	(iii)
11111000011111000011111000011110000011110000011110000011110000011110000	−9	(ii)
10000011111000001111100000111110000011111000001111100000111110000001111	+10	(ii)
11110001110001111000111000111000011100011100001110001110000111000111000	−13	(ii)
10000000111111100000001111111000000011111110000000111111100000000111111	+14	(ii)
11100111001100011001110011000110001100111001100011000110011100110001100	−19	(ii)
10101001010010101101011010100101001010110101101010010100101001010101101	+22	(iii)

$n = 36$	λ^e	usable
1111111111111111111111111111111111110000000000000000000000000000000000000	+1	(ii) R
1010101010101010101010101010101010101010101010101010101010101010101010100	+2	(iii)
1001100110011001100110011001100110011001100110011001100110011001100110001	+4	(ii)
1000111000111000111000111000111000111000111000111000111000111000111000011	+6	(ii)
1000011110000111100001111000011110000111100001111000011110000111100000111	+8	(ii)
1000000111111000000111111000000111111000000111111000000111111000000011111	+12	(ii)
1000000000111111111000000000111111111000000000111111111000000000011111111	+18	(ii)
1111110000011111000001111100000011111000001111100000011111000001111100000	−21	(ii)

$n = 37$	λ^e	usable
111111111111111111111111111111111111100000000000000000000000000000000000000	+1	(ii) R
101010101010101010101010101010101010101010101010101010101010101010101010100	+2	(iii)
111001110011100111001110011100111000110001100011000110001100011000110001100	−5	(ii)
111000110011100011001110001100111000110011100011001110001100111000110001100	+10	(ii)
110100101011010010101101001010110100101011010010101101001010110100101001010	+10	(iii)
100110001100111001100011001110011000110011100110001100111001100110000110011	+14	(ii)
111111110000000111111110000000011111110000000011111110000000011111110000000	−15	(ii)
111111101000000011111110100000011111110100000011111110100000011111110100000	+30	(ii)

$n = 38$	λ^e	usable
11111111111111111111111111111111111111000000000000000000000000000000000000000	+1	(ii) R
10101010101010101010101010101010101010101010101010101010101010101010101010100	+2	(iii)
10011001100110011001100110011001100110011001100110011001100110011001100110001	+4	(ii)
11110001111000111100011110001111000011100001110000111000011100001110000111000	−7	(ii)
11101001110100111010011101001110100011010001101000110100011010001101000110100	−7	(ii)
11010101101010110101011010101101010010101001010100101010010101001010100101010	−7	(iii)
11111000000111110000001111100000001111100000011111000000111110000001111100000	−11	(ii)
11110000111000111100001110001111000011100011110000111000111100001110000111000	+14	(ii)
11101000110100111010001101001110100011010011101000110100111010001101000110100	+14	(ii)
11010100101010110101001010101101010010101011010100101010110101001010100101010	+14	(iii)