A PASCAL-LIKE BOUND FOR THE NUMBER OF NECKLACES WITH FIXED DENSITY

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Abstract. A bound resembling Pascal’s identity is presented for binary necklaces with fixed density using Lyndon words with fixed density. The result is generalized to $k$-ary necklaces and Lyndon words with fixed content. The bound arises in the study of Nichols algebras of diagonal type.

1. INTRODUCTION

A necklace is the lexicographically smallest word in an equivalence class of words under rotation. A Lyndon word is a primitive necklace, which means that it is strictly smaller than any of its non-trivial rotations. The density of a binary word is the number of 1s it contains. Let $N(n, d)$ denote the set of all binary necklaces of length $n$ and density $d$. Similarly, let $L(n, d)$ denote the set of all binary Lyndon words of length $n$ and density $d$. Let the cardinality of these two sets be denoted by $N(n, d)$ and $L(n, d)$, respectively. The following formulae are well-known for any $n \geq 1$ and $0 \leq d \leq n$ (see [4] and [10, Sect. 2]):

$$N(n, d) = \frac{1}{n} \sum_{j \mid \gcd(n, d)} \phi(j) \left( \frac{n}{j} \right), \quad L(n, d) = \frac{1}{n} \sum_{j \mid \gcd(n, d)} \mu(j) \left( \frac{n}{j} \right),$$

where $\phi$ and $\mu$ denote Euler’s totient function and the Möbius function, respectively. Note that $N(n, d) = N(n, n-d)$ and $L(n, d) = L(n, n-d)$. Our main result is to prove the following Pascal’s identity-like bound on $N(n, d)$.

**Theorem 1.1.** For any $0 < d < n$,

$$N(n, d) \leq L(n-1, d) + L(n-1, d-1).$$

Bounds on necklaces and Lyndon words like the one presented in the above theorem are generally difficult to prove directly from their enumeration formulae. Previous bounds on these objects used in algorithm analysis [10] use a combinatorial-style proof, and that is the approach we follow in this paper. To prove this theorem, we actually show something stronger. Let $\Sigma_k = \ldots$
\{0,1,2,\ldots,k-1\} denote an alphabet of size \(k\). Let \(W_k(n_0,n_1,\ldots,n_{k-1})\) denote the set of all words over \(\Sigma_k\) where each symbol \(i\) appears precisely \(n_i\) times. Such a set is said to be a set with fixed content, as used by \[1,\text{ Sect. 18.3.3}\]. In a similar manner let \(N_k(n_0,n_1,\ldots,n_{k-1})\) denote the set of necklaces with the given fixed content and let \(L_k(n_0,n_1,\ldots,n_{k-1})\) denote the set of Lyndon words with the given fixed content. Let the cardinality of these two sets be denoted by \(N_k(n_0,n_1,\ldots,n_{k-1})\) and \(L_k(n_0,n_1,\ldots,n_{k-1})\), respectively. In \[4\] and \[10,\text{ Sect. 2}\], explicit formulas for the number of necklaces and Lyndon words with fixed content are given:

\[
N_k(n_0,n_1,\ldots,n_{k-1}) = \frac{1}{n} \sum_{j \mid \gcd(n_0,\ldots,n_{k-1})} \phi(j) \frac{(n/j)!}{(n_0/j)! \cdots (n_{k-1}/j)!},
\]

\[
L_k(n_0,n_1,\ldots,n_{k-1}) = \frac{1}{n} \sum_{j \mid \gcd(n_0,\ldots,n_{k-1})} \mu(j) \frac{(n/j)!}{(n_0/j)! \cdots (n_{k-1}/j)!},
\]

where \(n = n_0 + n_1 + \cdots + n_{k-1}\). In Section 3, we prove the following more general result.

**Theorem 1.2.** Let \(k \geq 2\) and \(n_0,n_1,\ldots,n_{k-1} \geq 1\) be positive integers. Then

\[
N_k(n_0,\ldots,n_{k-1}) \leq \sum_{i=0}^{k-1} L_k(n_0,\ldots,n_{i-1},n_i-1,n_{i+1},\ldots,n_{k-1}).
\]

Moreover, the inequality is strict if \(k > 2\).

Observe that when \(k = 2\), Theorem 1.2 simplifies to Theorem 1.1. After presenting some preliminary materials in Section 2, we prove the theorems in Section 3. For more background on Lyndon words see \[6\].

### 1.1. An Application

The inequalities in Theorems 1.1 and 1.2 seem to be new. They arised with the study of Nichols algebras of diagonal type in \[5\] in order to determine whether such a Nichols algebra is a free algebra. Roughly, the inequality implies that a certain rational function is in fact a polynomial, and freeness of the Nichols algebra holds if none of these polynomials vanish at the point of an affine space determined by the braiding of the Nichols algebra. The calculation of the zeros of such a polynomial simplifies significantly if the inequality is known to be strict. Strictness when \(k = 2\) is further discussed in Section 4.

### 2. Background

A word is called a prenecklace, if it is the prefix of some necklace. For any non-empty word \(\alpha\) let \(\text{lyn}(\alpha)\) be the length of the longest prefix of \(\alpha\) that is a Lyndon word. The following theorem was named the Fundamental
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Theorem of necklaces by Ruskey and a proof of the theorem is presented in [9] which builds on a foundation of results from Duval [3]. There is a similar statement by Reutenauer [8] on page 164.

Theorem 2.1. [2, Thm. 2.1] Let $\alpha = a_1 \cdots a_{n-1}$ be a prenecklace over the alphabet $\Sigma_k$, where $n, k \geq 2$. Let $p = \text{lyn}(\alpha)$ and let $b \in \Sigma_k$. Then $\alpha b$ is a prenecklace if and only if $a_{n-p} \leq b$. In this case,

$$\text{lyn}(\alpha b) = \begin{cases} p & \text{if } b = a_{n-p}, \\ n & \text{if } b > a_{n-p}. \end{cases}$$

The following corollaries follow immediately from the previous theorem.

Corollary 2.2. If $\alpha = a_1 a_2 \cdots a_n$ is a prenecklace and $b > a_n$, then the word $a_1 a_2 \cdots a_{n-1} b$ is a Lyndon word.

Corollary 2.3. If $\alpha = a_1 a_2 \cdots a_n$ is a necklace and $b > a_1$, then $\alpha b$ is a Lyndon word.

The following result also follows from the above theorem and corresponds to [2, Lem. 2.3].

Corollary 2.4. Let $\alpha = a_1 a_2 \cdots a_n$ be a prenecklace with $p = \text{lyn}(\alpha) < n$, that is, $\alpha$ is not a Lyndon word. Then $\alpha = (a_1 a_2 \cdots a_p)^j a_1 a_2 \cdots a_i$ for some $j \geq 1$ and $1 \leq i \leq p$. Moreover, these $j$ and $i$ are uniquely determined.

The following remark follows directly from the definition of a necklace.

Remark 2.5. Every necklace over $\Sigma_k$ that contains a 0 and a non-0 element must begin with 0 and end with a non-0.

3. Proof of Main Theorems

A necklace $\alpha = a_1 a_2 \cdots a_n$ is said to be stable if $a_1 a_2 \cdots a_{n-1}$ is a Lyndon word; otherwise $\alpha$ is unstable. We prove Theorem 1.2, which generalizes Theorem 1.1, by partitioning $N_k(n_0, n_1, \ldots, n_{k-1})$ into two sets $S$ and $U$, which contain the stable and unstable necklaces of $N_k(n_0, n_1, \ldots, n_{k-1})$, respectively.

Lemma 3.1. Let $k \geq 2$ and $n_0, n_1, \ldots, n_{k-1} \geq 1$ be positive integers. Then

$$|S| = \sum_{i=1}^{k-1} L_k(n_0, \ldots, n_{i-1}, n_i-1, n_{i+1}, \ldots, n_{k-1}).$$

Proof. Since each $n_i > 0$, by Remark 2.5 every necklace in $S$ must begin with 0 and end with a non-0. By partitioning $S$ by its last symbol, the result follows from Corollary 2.3 and the definition of stable. \qed
It remains to show that $|U| \leq L_k(n_0-1, n_1, n_2, \ldots, n_{k-1})$. We assume $k \geq 2$ and each $n_i \geq 1$. Let $\alpha = a_1a_2 \cdots a_n$ be a necklace in $U$. From Remark 2.5, $a_1 = 0$ and $a_n > 0$. Let $\alpha' = a_1a_2 \cdots a_{n-1}$ and let $x = a_n$. Since $\alpha$ is unstable, $\alpha'$ is a prenecklace, but not a Lyndon word. Thus, applying Corollary 2.4, we can write $\alpha = (a_1a_2 \cdots a_n)^j a_1a_2 \cdots a_i$ where $j \geq 1$ and $1 \leq i \leq p$. Define $\beta$, which we call the index of $\alpha$ associated with $f$, to be the largest index no more than $i$ such that $a_z = 0$. Such an index exists since $a_1 = 0$. Thus

$$\alpha = (a_1a_2 \cdots a_p)^j a_1a_2 \cdots a_{z-1}a_z a_{z+1} \cdots a_i x.$$  

Consider the function $f : U \to L_k(n_0-1, n_1, n_2, \ldots, n_{k-1})$ as follows:

$$f(\alpha) = \begin{cases} (a_1a_2 \cdots a_p)^j a_1a_2 \cdots a_z x & \text{if } z = i; \\ (a_1a_2 \cdots a_p)^j x a_i a_{i-1} \cdots a_z + 2 a_1 a_2 \cdots a_z - 1 a_z + 1 & \text{if } z < i. \end{cases}$$

Clearly $f(\alpha)$ has the required content. To see that $f(\alpha)$ is a Lyndon word, consider two cases depending on $z$. Suppose $z = i$. Then since $\alpha$ is a necklace, $(a_1a_2 \cdots a_p)^j a_1a_2 \cdots a_z$ is a prenecklace. Thus since $x > a_z$, $(a_1a_2 \cdots a_p)^j a_1a_2 \cdots a_z x$ is a Lyndon word by Corollary 2.2. Suppose $z < i$. Note that $(a_1a_2 \cdots a_p)^j$ is a necklace and $a_1 = 0$. Since each symbol in $xa_i a_{i-1} \cdots a_z + 2$ is non-zero, $\beta = (a_1a_2 \cdots a_p)^j x a_i a_{i-1} \cdots a_z + 2$ is a Lyndon word by Corollary 2.3. Observe that $\beta a_1a_2 \cdots a_z$ is a prenecklace, since it is a prefix of the necklace $\beta^2$. Thus, since $a_{z+1} > 0$ from the definition of $z$ and $a_z = 0$, Corollary 2.2 implies $\beta a_1a_2 \cdots a_z - 1 a_z + 1$ is a Lyndon word. Hence $f(\alpha)$ is a Lyndon word.

**Lemma 3.2.** Let $k \geq 2$ and $n_0, n_1, \ldots, n_{k-1}$ be positive integers. Then

$$|U| \leq L_k(n_0-1, n_1, n_2, \ldots, n_{k-1}).$$

**Proof.** We prove that $f$ is one-to-one. Consider necklaces $\alpha$ and $\beta$ in $U$. Set:

$$\alpha = (a_1a_2 \cdots a_p)^j a_1a_2 \cdots a_z a_{z+1} a_{z+2} \cdots a_i x,$$

$$\beta = (b_1b_2 \cdots b_{p'})^{j'} b_1 b_2 \cdots b_{z'-1} b_z b_{z'+1} b_{z'+2} \cdots b_{p'} x'.$$

where $z$ (resp. $z'$) is the index of $\alpha$ (resp. of $\beta$) associated with $f$. Suppose $f(\alpha) = f(\beta)$. If $j p = j' p'$, then $p = p'$ since both $a_1a_2 \cdots a_p$ and $b_1 b_2 \cdots b_{p'}$ are Lyndon words. If $p = p'$ then clearly $\alpha = \beta$ by the definition of $f$. Thus, without loss of generality assume that $j p < j' p'$. Suppose $p < p' < j p$, which implies $j > 1$. But this implies there exists $1 \leq h < j$ and $0 < t \leq p$ such that $b_1 b_2 \cdots b_{p'} = (a_1a_2 \cdots a_p)^h a_1 a_2 \cdots a_t$ which contradicts $b_1 b_2 \cdots b_{p'}$ being a Lyndon word. By a similar argument we cannot have $p' < p \leq j' p'$. Thus $j p < p'$, which by the definition of $f$, implies $j' = 1$ and $a_1 a_2 \cdots a_p = b_1 b_2 \cdots b_{p'}$. Consider two cases based on $\ell = |a_{z+2} \cdots a_i x|$.
(i) Suppose $jp + \ell \geq p'$. This implies $\ell > 0$. Let $\ell' = |b_{\ell'+1} \cdots b_{\ell+1}x'|$. Recall $a_1 = b_1 = 0$ and each letter of $a_{z+1} \cdots a_1x$ and $b_{\ell'+1} \cdots b_{\ell+1}x'$ is non-0. Thus, since $f(\alpha) = f(\beta)$, we must have $jp + \ell = p' + \ell'$, which means $z = z'$. But this means $x' = a_{\ell'+1} = b_{\ell+1}$, which means that $\beta$ ends with $b_1b_2 \cdots b_{\ell+1}$ which is a proper prefix of $b_1b_2 \cdots b_{\ell'}$, contradicting $\beta$ being a necklace.

(ii) Suppose $jp + \ell < p'$. In this case, for $f(\alpha) = f(\beta)$, it must be that some suffix of $b_1b_2 \cdots b_{\ell'}$ is a prefix of $a_1a_2 \cdots a_{z-1} = b_1b_2 \cdots b_{z-1}$ which contradicts $b_1b_2 \cdots b_{\ell'}$ being a Lyndon word.

□

Together Lemma 3.1 and Lemma 3.2 prove Theorem 1.1. To complete the proof of Theorem 1.2, the following lemma proves that for $k > 2$ the function $f$ is not a bijection.

**Lemma 3.3.** The function $f$ is not a surjection when $k > 2$.

**Proof.** We consider two cases depending on the parity of $n_0$. For each case we demonstrate a word $\gamma$ in $L_k(n_0-1, n_1, n_2, \ldots, n_{k-1})$ that is not in the range of $f$. Observe that if $\alpha \in U$ such that $f(\alpha) = \gamma$, and $\alpha \neq 0^m x$ for some $m > 0$, $x \in \Sigma_k$, then the shortest prefix $u$ of $\gamma = uv$ containing two different symbols is a prefix of $\alpha$. Moreover, if $v$ ends with $0^j t$, with $j \geq 0$ and $t \in \{1, 2, \ldots, k-1\}$, then $0^{j+1} t$ is a subword of $\alpha$.

- Case 1: $n_0 = 2j + 1$ for $j \geq 0$. There is no necklace in $U$ that maps to the Lyndon word $0^j 1^{n_1} 2^{n_2} \cdots (k-1)^{n_{k-1}-1} 0^{j'(k-1)}$ because such a necklace would have to start with $0^{j'} 1$ but have the subword $0^{j'+1}$.

- Case 2: $n_0 = 2j$ for $j \geq 1$. There is no necklace in $U$ that maps to the Lyndon word $0^{j'(k-1)} 3^{n_1} 2^{n_2} 1^{n_{k-1}-1} 0^{j-1}$ because such a necklace would have to start with $0^{j'(k-1)}$ but have the subword $0^{j'} 1$.

□

4. Special Cases When $N(n, d) = L(n-1, d) + L(n-1, d-1)$

In this section we discuss when the inequality given by Theorem 1.1 is equality. Recall that the density $d$ of a binary word is the number of 1s it contains.

**Lemma 4.1.** If $d \in \{1, 2, n-2, n-1\}$ and $0 < d < n$ then $N(n, d) = L(n-1, d) + L(n-1, d-1)$ except for $(n, d) = (2, 1)$.

**Proof.** Recall that $N(n, d) = N(n, n-d)$ and $L(n, d) = L(n, n-d)$. Thus it suffices to prove the result for $d = 1$ and $d = 2$. For $d = 1$ and $n > 2$, $N(n, 1) = \{0^{n-1} 1\}$, $L(n-1, 1) = \{0^{n-2} 1\}$, and $L(n-1, 0) = \emptyset$, and thus
the result holds. For \( d = 2 \), consider the parity of \( n \). If \( n \) is even, then \( \mathbf{L}(n, 2) = \{0^{n-j-2}10^j \mid j \in \{0, 1, \ldots, \frac{n-2}{2} - 1\} \} \) and \( \mathbf{N}(n, 2) = \mathbf{L}(n, 2) \cup \{0^{(n-2)/2}10^{(n-2)/2}\} \). If \( n \) is odd, then \( \mathbf{N}(n, d) = \mathbf{L}(n, 2) = \{0^{n-j-2}10^j \mid j \in \{0, 1, \ldots, \frac{n-3}{2}\} \} \). Thus, \( \mathbf{N}(n, 2) = \left\lceil \frac{n}{2}\right\rceil \), \( \mathbf{L}(n-1, 2) = \left\lceil \frac{n-2}{2}\right\rceil \), and \( \mathbf{L}(n-1, 1) = 1 \), and therefore the result holds.

We now consider the other values of \( d \).

**Lemma 4.2.** If \( 2 < d < n - 2 \) then \( \mathbf{N}(n, d) = \mathbf{L}(n-1, d) + \mathbf{L}(n-1, d-1) \) if and only if \( (n, d) \in \{(6, 3), (7, 3), (7, 4), (8, 4), (9, 3), (9, 6)\} \).

**Proof.** The claim can be verified directly from the enumeration formulae for \( n \leq 10 \). A table of relevant values for \( \mathbf{N}(n, d) \) (resp. \( \mathbf{L}(n, d) \)) are provided in the left (resp. right) table below.

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<tr>
<th>( n/d )</th>
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For \( n > 10 \), let \( z = n - d \) (the number of 0s). Recall that \( \mathbf{N}(n, d) = \mathbf{N}(n, n-d) \) and \( \mathbf{L}(n, d) = \mathbf{L}(n, n-d) \). Thus, if \( \mathbf{N}(n, d) = \mathbf{L}(n-1, d) + \mathbf{L}(n-1, d-1) \) then \( \mathbf{N}(n, n-d) = \mathbf{L}(n-1, n-d) + \mathbf{L}(n-1, n-(d-1)) \). Thus, we can assume \( 2 < z \leq n/2 \). Consider three cases for \( z = 3, z = 4, \) and \( z \geq 5 \). Each result is proved by specifying a Lyndon word \( \beta \in \mathbf{L}(n-1, d) = \mathbf{L}_2(z-1, d) \) not in the range of \( f \) when the domain is the set of unstable necklaces in \( \mathbf{N}(n, d) = \mathbf{N}_2(z, d) \).

- **Case:** \( z = 3 \). Depending on the parity of \( n \) let \( \beta \) be either \( 01^a01^{a+1} \) or \( 01^a01^{a+2} \). Since \( n > 10, a \geq 3 \). Consider any necklace \( \alpha \) in \( \mathbf{N}_2(3, d) \) which can be written as \( 01^a01^{a+1}a \) for non-negative integers \( a_1, a_2, a_3 \). Note that if \( a_2 < a_1 \) then the the rotation of \( \alpha \) starting with \( 01^{a_2} \) is less than \( \alpha \), a contradiction to \( \alpha \) being a necklace. Similarly for \( a_3 \). Thus, \( a_2, a_3 \geq a_1 \). But for any such (unstable) \( \alpha \), \( f(\alpha) = 01^a01^{a+2+a_3} \neq \beta \).

- **Case:** \( z = 4 \). Depending on the value of \( (n \mod 3) \) let \( \beta \) be one of the words \( 01^a01^{a+1}, 01^a01^{a+1}01^{a+1}, \) and \( 01^a01^{a+1}01^{a+2} \). Since \( n > 10, a \geq 2 \). Consider any necklace \( \alpha \) in \( \mathbf{N}_2(4, d) \) which can be written as \( 01^a01^{a+1}01^{a+1}a \) for non-negative integers \( a_1, a_2, a_3, a_4 \). Since \( \alpha \) is a necklace and \( n > 10, a_4 > 1 \). Again, observe that if \( a_2 < a_1 \) then the the rotation of \( \alpha \) starting with \( 01^{a_2} \) is less than \( \alpha \), a contradiction to \( \alpha \) being a necklace. Similarly for \( a_3, a_4 \). Thus, \( a_2, a_3, a_4 \geq a_1 \). Recall we can write \( \alpha \) as \( (a_1a_2\cdots a_p)\beta a_1a_2\cdots a_i\beta' \) for some
where \( x = 1, j \geq 1, \) and \( 1 \leq i \leq p \) where \( p \) is the longest Lyndon prefix of \( \alpha \). Thus, either \( p = a_1 + a_2 + 2 \) or \( p = a_1 + a_2 + a_3 + 3 \). In the first case, we must have \( a_2 > a_3 \), since \( a_1 a_2 \cdots a_p \) is a Lyndon word. Thus since \( a_4 > 1 \), we have \( f(\alpha) = 01^{a_1}01^{a_2 + a_4 - 1}01^{a_3 + 1} \). In the latter case, \( f(\alpha) = 01^{a_1}01^{a_2}01^{a_3 + a_4} \). Neither case is equal to \( \beta \).

- Case: \( z \geq 5 \). Recall \( n > 10 \) and \( z \leq n/2 \). Consider the length \( n \) word \( \beta = 001^z01(01)^b \) where \( b = z - 4 \) and \( a = n - 2b - 5 \). Since \( z \geq 5, b \geq 1 \) Clearly \( \beta \) is a Lyndon word and it has \( z - 1 \) 0s. Now suppose there exists an unstable necklace \( \alpha = a_1 a_2 \cdots a_n \) in \( N_2(z, d) \) such that \( f(\alpha) = \beta \). Recall we can write \( \alpha \) as \( (a_1 a_2 \cdots a_p)^j a_1 a_2 \cdots a_i x \) where \( x = 1, j \geq 1, \) and \( 1 \leq i \leq p \). As noted earlier, if \( \beta \) begins with 001, then so must \( \alpha \). Thus \( a_1 a_2 a_3 = 001 \). Consider \( z \), the index of \( \alpha \) associated with \( f \). If \( z > 2 \), then \( f(\alpha) \) must have two subwords of the form 001 and hence is not equal to \( \beta \). Otherwise \( z = 2 \). If \( i = z \) then \( \alpha \) ends with 001. In order for \( f(\alpha) = \beta, \) \( \alpha \) must begin with 0011. However this contradicts \( \alpha \) being a necklace. Thus \( z < i \). However, in this case \( f(\alpha) \) must end 1101 which contradicts \( \beta \) ending with 0101.

\[ \square \]

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