A New Shuffle Convolution for Multiple Zeta Values

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Abstract. Recently, interest in shuffle algebra has been renewed due to their connections with multiple zeta values. In this paper, we prove a new shuffle convolution that implies a reduction formula for the multiple zeta value $\zeta(\{5, 1\}^n)$.

1. Introduction

As in [4, 5, 7], let X be a finite set and let X^* denote the free monoid generated by X. We can regard X as an alphabet, and the elements of X^* as words formed by concatenating any finite number of letters (repetitions permitted) from X.

With the empty word denoted by 1, it is now possible to define the shuffle product by the recursion

$$\begin{cases} \forall w \in X^*, & 1 \sqcup\!\sqcup w = w \sqcup\!\sqcup 1 = w, \\ \forall a, b \in X, \quad \forall u, v \in X^*, & au \sqcup\!\sqcup bv = a(u \sqcup\!\sqcup bv) + b(au \sqcup\!\sqcup v). \end{cases} \tag{1}$$

We can easily see that the shuffle product is associative and commutative.

On the other hand, the shuffle product can be defined in terms of permutations. For non-negative integers m and n, let $\mathrm{Shuff}(m, n)$ denote the set of all $\binom{m+n}{n}$ permutations σ of the index set $\{1, 2, \ldots, m + n\}$ that satisfy $\sigma^{-1}(j) < \sigma^{-1}(k)$ for all $1 \le j < k \le m$ and $m + 1 \le j < k \le m + n$. Then, the shuffle recursion (1) is easily seen to be equivalent to

$$\left(\prod_{j=1}^{m} x_j \right) \sqcup\!\sqcup \left(\prod_{j=m+1}^{m+n} x_j \right) := \sum_{\sigma \in \mathrm{Shuff}(m,n)} \prod_{j=1}^{m+n} x_{\sigma(j)}, \quad x_j \in X. \tag{2}$$

The sum (2) is over all non-commutative products (counting multiplicity) of length $m + n$ in which the relative orders of the factors in the products $x_1 \cdots x_m$ and $x_{n+1} \cdots x_{m+n}$ are preserved. The term "shuffle" is used because such permutations arise in riffle shuffling a deck of $m + n$ cards cut into one pile of m cards and a second pile of n cards. Throughout this paper, we will adopt this definition of the shuffles.

Interest in shuffles has been renewed due to their intimate connections with multiple zeta values [1, 2, 5–10, 12] and multiple polylogarithms [3, 4, 13]. For example, in [2] it was shown that the shuffle convolution formula

$$\sum_{r=-n}^{n} (-1)^r [(ab)^{n-r} \; \sqcup\!\sqcup \; (ab)^{n+r}] = (4a^2b^2)^n, \qquad 0 \le n \in \mathbb{Z},$$

implies the evaluation

$$\zeta(\{3, 1\}^n) := \zeta(\underbrace{3, 1, \ldots, 3, 1}_{2n \text{ arguments}}) = \frac{2\pi^{4n}}{(4n+2)!}, \qquad 0 \le n \in \mathbb{Z},$$

for the multiple zeta function defined by

$$\zeta(s_1, \ldots, s_k) := \sum_{n_1 > \cdots > n_k > 0} \prod_{j=1}^{k} n_j^{-s_j}.$$

The primary purpose of this paper is to prove a conjecture of D. Bowman on shuffles (Conjecture 1 below). It follows from our proof of Conjecture 1 that (communication from Bowman)

$$\zeta(\{5, 1\}^n) := \zeta(\underbrace{5, 1, \ldots, 5, 1}_{2n \text{ arguments}}), \qquad 0 \le n \in \mathbb{Z},$$

can be explicitly evaluated. Unfortunately, this evaluation has not been communicated to us.

Let n be a positive integer. We begin by observing that in $(a^4b^2)^n$, every occurrence of a^4 after the first is separated on both sides by b^2, and hence there are $2n - 1$ ways in which a single transposition of a letter b with an adjacent letter a can be performed. If we let

$$\Xi_n(k)$$

denote the sum of the $\binom{2n-1}{k}$ words obtained from $(a^4b^2)^n$ by making k such transpositions, then we have the following result.

Conjecture 1 (D. Bowman) *Let n be a positive integer. Then*

$$\sum_{r=-n}^{n} (-1)^r [(a^2b)^{n-r} \; \sqcup\!\sqcup \; (a^2b)^{n+r}] = 3^n \sum_{k=0}^{2n-1} 2^{2n-k} \, \Xi_n(k). \qquad (3)$$

Example. When $n = 2$, the right hand side of Theorem 1 is equal to

$$3^2 \sum_{k=0}^{3} 2^{4-k} \Xi_2(k) = 144a^4b^2a^4b^2 + 72(a^4b^2a^3bab + a^4baba^3b^2 + a^3baba^4b^2)$$
$$+ 36(a^3baba^3bab + a^3ba^2ba^3b^2 + a^4baba^2bab) + 18a^3ba^2ba^2bab,$$

which implies that

$$144\zeta(\{5, 1\}^2) = \sum_{r=-2}^{2} (-1)^r \zeta(\{3\}^{2-r})\zeta(\{3\}^{2+r}) - 72(\zeta(5, 1, 4, 2) + \zeta(5, 2, 4, 1)$$
$$+ \zeta(4, 2, 5, 1)) - 36(\zeta(4, 2, 4, 2) + \zeta(4, 3, 4, 1) + \zeta(5, 2, 3, 2))$$
$$-18\zeta(4, 3, 3, 2). \tag{4}$$

The identity (4) is a special case of (12) below.

In Section 2, we present notation and establish some propositions which we use throughout this paper. Conjecture 1 is proved and restated in terms of multiple zeta values in Section 3.

2. Preliminaries

Before proving the shuffle convolution formula (3), we need to establish some additional notation and results.

Henceforth, we adopt the convention that concatenation takes precedence over the shuffle operation, so that in (2) the parentheses can be omitted. Also, it will be convenient to denote the multi-set of words arising in the shuffle product (2) by

$$\{x_1 \cdots x_m \sqcup\!\sqcup x_{m+1} \cdots x_{m+n}\}.$$

For example, $\{ab \sqcup\!\sqcup a\} = \{aba, aab, aab\}$. From (2), it is clear that to every distinct word

$$w \in \left\{ \prod_{j=1}^{m} x_j \sqcup\!\sqcup \prod_{j=m+1}^{m+n} x_j \right\},$$

there corresponds at least one permutation $\sigma \in \text{Shuff}(m, n)$ such that

$$w = \prod_{j=1}^{m+n} x_{\sigma(j)}.$$

We call such a permutation σ *a shuffle corresponding to* w.

In [11], D. Loeb introduced hybrid sets, which is defined as follows.

Definition 1 (D. Loeb [11])   Given a universe U, any function $f : U \to \mathbb{Z}$ is called a hybrid set. The value of $f(x)$ is said to be the multiplicity of the element x. If $f(x) \neq 0$, we say x is a member of f and write $x \in f$; otherwise, we write $x \notin f$. Define the number of elements $\#f$ to be the sum $\sum_{x \in U} f(x)$. Then f is said to be an $\#f$ hybrid set.

Hybrid sets are denoted by $\{ \mid \}$, where elements occurring with positive multiplicities are written on the right of the bar, and elements occurring with negative multiplicities are written on the left. Order is completely irrelevant. For example, if $f = \{d, e, e \mid a, b, c, b\}$, then $f(a) = 1$, $f(b) = 2$, $f(c) = 1$, $f(d) = -1$, $f(e) = -2$, and $f(x) = 0$ for $x \neq a, b, c, d, e$.

Note that in Loeb's paper, elements occurring with positive multiplicities appear on the left of the bar and elements occurring with negative multiplicities appear on the right of the bar, but we follow the definition above throughout this paper.

Loeb did not discuss the product of hybrid sets. We define the product of hybrid sets as follows.

Definition 2   Consider two hybrid sets $f : U \to \mathbb{Z}$ and $g : V \to \mathbb{Z}$. We define the product $U \times V$ of U and V as the set of elements obtained by concatenating $x \in U$ and $y \in V$, i.e.,

$$U \times V = \{xy : x \in U, y \in V\}.$$

The product $f \times g$ of f and g is a hybrid set from $U \times V$ to $\mathbb{Z}$ defined by

$$f \times g\,(xy) = f(x)g(y),$$

where $x \in f$ and $y \in g$.

From the definition of the number of elements of a hybrid set, the number of elements $\#f \times g$ is defined by

$$\#(f \times g) = \sum_{xy \in U \times V} f \times g(xy),$$

which is equal to

$$\sum_{x \in U,\ y \in V} f(x)g(y) = \sum_{x \in U} f(x) \sum_{y \in V} g(y) = (\#f)(\#g).$$

Similarly, we can generalize the product of two hybrid sets to more than two hybrid sets.

If w is any word, let $|w|$ denote its length, that is, the number of letters in w, counting multiplicity. For $w \in \{a, b\}^*$, we denote the number of occurrences of the letter a in w by $|w|_a$. Similarly, the number of occurrences of the letter b in w is denoted by $|w|_b$, so that $|w| = |w|_a + |w|_b$. For $1 \leq j \leq |w|_b$, let $b_j = b_j(w)$ be the jth b from the left; let $a(1)$ be the number of times the letter a occurs to the left of b_1; and for $1 < j \leq |w|_b$ let $a(j)$ be the number of times the letter a occurs between b_{j-1} and b_j. Let $A(w)$ denote the sequence $a(1), a(2), \ldots, a(|w|_b)$.

Proposition 1 *Let X be an alphabet, let m and n be non-negative integers, and let*

$$w \in \left\{ \prod_{j=1}^{m} x_j \ \text{ш} \ \prod_{j=m+1}^{m+n} x_j \right\}, \qquad x_j \in X.$$

If k is an integer such that $0 \leq k \leq m + n$, and $w = uv$ with $|u| = k$, then there exist non-negative integers m_1 and n_1 satisfying $m_1 + n_1 = k$ and such that

$$u \in \left\{ \prod_{j=1}^{m_1} x_j \ \text{ш} \ \prod_{j=m_1+1}^{m_1+n_1} x_{m-m_1+j} \right\} \tag{5}$$

and

$$v \in \left\{ \prod_{j=1}^{m-m_1} x_{m_1+j} \ \text{ш} \ \prod_{j=m-m_1+1}^{m-m_1+n-n_1} x_{m_1+n_1+j} \right\}. \tag{6}$$

Conversely, given non-negative integers m_1, m_2, n_1, and n_2, let

$$u \in \left\{ \prod_{j=1}^{m_1} x_j \ \text{ш} \ \prod_{j=m_1+1}^{m_1+n_1} x_j \right\} \quad and \quad v \in \left\{ \prod_{j=1}^{m_2} y_j \ \text{ш} \ \prod_{j=m_2+1}^{m_2+n_2} y_j \right\}, \qquad x_j, \ y_j \in X.$$

Then

$$uv \in \left\{ \left(\prod_{j=1}^{m_1} x_j \right) \left(\prod_{j=1}^{m_2} y_j \right) \ \text{ш} \ \left(\prod_{j=m_1+1}^{m_1+n_1} x_j \right) \left(\prod_{j=m_2+1}^{m_2+n_2} y_j \right) \right\}. \tag{7}$$

Proof: Let σ be a shuffle corresponding to w. Then

$$u = \prod_{j=1}^{k} x_{\sigma(j)} \qquad and \qquad v = \prod_{j=k+1}^{m+n} x_{\sigma(j)}.$$

Let $m_1 = |\{j \in \mathbb{Z} : 1 \leq j \leq k, \sigma(j) \leq m\}|$, and put $n_1 = k - m_1$. Note that if $1 \leq j \leq k$ and $\sigma(j) \leq m$, then $\sigma(j) \leq m_1$, since $\sigma \in \text{Shuff}(m, n)$. Similarly, $1 \leq j \leq k$ and $m + 1 \leq \sigma(j) \leq m + n$ implies $m + 1 \leq \sigma(j) \leq m + n_1$. Hence, we can define a permutation τ on $\{1, 2, \ldots, k\}$ by

$$\tau(j) = \begin{cases} \sigma(j), & \text{if } 1 \leq \sigma(j) \leq m, \\ \sigma(j) - m + m_1, & \text{if } m + 1 \leq \sigma(j) \leq m + n. \end{cases}$$

Similarly, we can define a permutation ρ on $\{1, 2, \ldots, m + n - k\}$ by

$$\rho(j) = \begin{cases} \sigma(j + k) - m_1, & \text{if } 1 \leq \sigma(j + k) \leq m, \\ \sigma(j + k) - k, & \text{if } m + 1 \leq \sigma(j + k) \leq m + n. \end{cases}$$

Since $\sigma \in \text{Shuff}(m, n)$, we see that $\tau \in \text{Shuff}(m_1, n_1)$ and $\rho \in \text{Shuff}(m - m_1, n - n_1)$. Let $z_j = x_j$ for $1 \leq j \leq m_1$ and $z_j = x_{m-m_1+j}$ for $m_1 + 1 \leq j \leq m_1 + n_1$. Then

$$u = \prod_{j=1}^{k} z_{\tau(j)}.$$

Since $\tau \in \text{Shuff}(m_1, n_1)$, it follows that

$$u \in \left\{ \prod_{j=1}^{m_1} z_j \ \sqcup\!\sqcup \ \prod_{j=m_1+1}^{m_1+n_1} z_j \right\},$$

which is equivalent to (5). Similarly, we can show that ρ is a shuffle corresponding to v in the shuffle product (6).

For the converse, let $\tau \in \text{Shuff}(m_1, n_1)$ and $\rho \in \text{Shuff}(m_2, n_2)$ be shuffles corresponding to u and v, respectively. Then

$$u = \prod_{j=1}^{m_1+n_1} x_{\tau(j)} \quad \text{and} \quad v = \prod_{j=1}^{m_2+n_2} y_{\rho(j)}.$$

We define a permutation σ on $\{1, 2, \ldots, m_1 + n_1 + m_2 + n_2\}$ by

$$\sigma(j) = \begin{cases} \tau(j), & \text{if } 1 \leq \tau(j) \leq m_1, \\ \tau(j) + m_2, & \text{if } m_1 + 1 \leq \tau(j) \leq m_1 + n_1, \end{cases}$$

for $1 \leq j \leq m_1 + n_1$, and

$$\sigma(j) = \begin{cases} \rho(j - m_1 - n_1) + m_1, & \text{if } 1 \leq \rho(j - m_1 - n_1) \leq m_2, \\ \rho(j - m_1 - n_1) + m_1 + n_1, & \text{if } m_2 + 1 \leq \rho(j - m_1 - n_1) \leq m_2 + n_2, \end{cases}$$

for $m_1 + n_1 + 1 \leq j \leq m_1 + n_1 + m_2 + n_2$. Since $\tau \in \text{Shuff}(m_1, n_1)$ and $\rho \in \text{Shuff}(m_2, n_2)$, it follows that $\sigma \in \text{Shuff}(m_1 + m_2, n_1 + n_2)$. Let

$$z_j = \begin{cases} x_j, & \text{if } 1 \leq j \leq m_1, \\ y_{j-m_1}, & \text{if } m_1 + 1 \leq j \leq m_1 + m_2, \\ x_{j-m_2}, & \text{if } m_1 + m_2 + 1 \leq j \leq m_1 + m_2 + n_1, \\ y_{j-m_1-n_1}, & \text{if } m_1 + m_2 + n_1 + 1 \leq j \leq m_1 + m_2 + n_1 + n_2. \end{cases}$$

Then

$$uv = \prod_{j=1}^{m_1+n_1+m_2+n_2} z_{\sigma(j)}.$$

Since $\sigma \in \text{Shuff}(m_1 + m_2, n_1 + n_2)$,

$$uv \in \left\{ \prod_{j=1}^{m_1+m_2} z_j \, \sqcup\!\sqcup \, \prod_{j=m_1+m_2+1}^{m_1+m_2+n_1+n_2} z_j \right\},$$

which is equivalent to (7). $\square$

In the remainder of our paper, X has only two elements, a and b. We need to make further definitions, to study carefully the formation of words in the shuffle convolution (3), and to carefully examine words in X^*.

Definition 3 For a non-negative integer n, let Π_n be the set of all non-negative integer sequences $\pi = (\pi_1, \pi_2, \ldots, \pi_n)$ satisfying

$$2m \leq \sum_{j=1}^{m} \pi_j \leq 2m + 2 \quad \text{for} \quad m < n, \quad \text{and} \quad \sum_{j=1}^{n} \pi_j = 2n. \tag{8}$$

Proposition 2 *Let n and r be non-negative integers with $n \geq r$, and let*

$$w \in \{(a^2b)^r \, \sqcup\!\sqcup \, (a^2b)^{n-r}\}.$$

Then $A(w)$ belongs to Π_n.

Conversely, there exists a non-negative integer r with $r \leq n$ such that $w \in \{(a^2b)^{n-r} \, \sqcup\!\sqcup \, (a^2b)^r\}$ for $w \in \{a, b\}^*$, and $A(w)$ belongs to Π_n.

Proof: Let $n \geq r, 1 \leq m \leq n, u := (a^2b)^r$, and $v := (a^2b)^{n-r}$, and suppose $w \in \{u \, \sqcup\!\sqcup \, v\}$. Since each b in any power of a^2b is immediately preceded by two consecutive occurrences of the letter a, the shuffle rule (2) implies that the number of times the letter a appears to the left of b_m is at least $2m$. In other words,

$$2m \leq \sum_{j=1}^{m} a(j).$$

It is possible that there are up to two additional occurrences of the letter a preceding b_m. Let τ be the initial subword of w consisting of the letters from w_1 up to and including b_m. In the formation of τ, let k be the number of occurrences of the letter b that came from u; then the remaining $m - k$ came from v. If b_m came from u, then τ was formed from $(a^2b)^k \, \sqcup\!\sqcup \, (a^2b)^{m-k}s$, where s is either a, a^2, or the empty word. Similarly, if b_m

came from v, then τ was formed from $(a^2b)^m s \sqcup (a^2b)^{m-k}$. Since the letters of s could precede b_m in τ, it follows that

$$\sum_{j=1}^{m} a(j) \leq 2m + 2.$$

For the converse, first observe that if $w \in \{a, b\}^*$ satisfies $|w|_a = 2|w|_b = 2n$ and the system of inequalities (8) holds for $1 \leq m \leq n$, then $2 \leq a(1) \leq 4$ and $0 \leq a(m) \leq 4$ for $1 < m \leq n$. Suppose there are precisely s indices $m_1 < m_2 < \cdots < m_s$ satisfying $0 \leq a(m_k) \leq 1$ for $1 \leq k \leq s$. We may assume $s > 0$, for otherwise $|w|_a = 2|w|_b$ implies $w = (a^2b)^n$, and the conclusion is trivial. Since

$$2m_1 < \sum_{j=1}^{m_1} a(j) \leq 2m_1 + 2,$$

there exists $m < m_1$ for which $3 \leq p := a(m) \leq 4 - a(m_1)$. Choose the maximal such m, and remove $p - 2$ of the letters a that occur between b_{m-1} and b_m (before b_1 if $m = 1$), so that in the modified word, $a(m) = 2$. If $p = 4$, then two letters a are removed; let us also remove b_{m_1} so that a^2b has been removed. If $p = 3$, then only one letter a is removed, and either $a(m_1) = 1$, or there exists $m' < m$ for which $a(m') = 3$. Now remove also b_{m_1} and the a that immediately precedes b_{m_1} if $a(m_1) = 1$. Otherwise, remove b_{m_1} and the a that immediately precedes $b_{m'}$, so that now $a(m') = 2$. Then a^2b has been removed from w. Repeat the process for $m_2, \ldots, m_s$ until we get $(a^2b)^{n-r}$ left for some $r \leq s$. Note that $(a^2b)^r$ is removed from w and $w \in \{(a^2b)^r \sqcup (a^2b)^{n-r}\}$. $\square$

3.   The main result

Definition 4   For each non-negative integer n and each integer r with $|r| \leq n$, let

$$S_{n,r} := \{(a^2b)^{n-r} \sqcup (a^2b)^{n+r}\} \qquad \text{and} \qquad S_n := \{\cup_{r \text{ odd}} S_{n,r} \mid \cup_{r \text{ even}} S_{n,r}\}.$$

Definition 5   For a non-negative integers n, let Δ_n be the subset of Π_{2n} such that

$$\begin{cases} 2m+1 \leq \sum_{j=1}^{m} \pi_j \leq 2m+2, & \text{if } m \text{ is odd,} \\[2mm] 2m \leq \sum_{j=1}^{m} \pi_j \leq 2m+1, & \text{if } m \text{ is even and less than } 2n, \\[2mm] \sum_{j=1}^{2n} \pi_j = 4n, & \text{if } m = 2n, \end{cases} \qquad (9)$$

and for a non-negative integer k, let $\Delta_n(k)$ be the subset of Δ_n such that

$$e(\pi) := \pi_2 + \pi_4 + \cdots + \pi_{2n} = k. \qquad (10)$$

Since (9) implies $0 \le \pi_{2m} \le 2$ for any $m < n$ and $0 \le \pi_{2n} \le 1$, we see that $\Delta_n(k)$ is empty if $k \ge 2n$. In other words, we partition Δ_n into $2n$ subsets $\Delta_n(k)$,

$$\Delta_n = \bigcup_{k=0}^{2n-1} \Delta_n(k). \tag{11}$$

Example. When $n = 2$,

$$\Delta_2(0) = \{(4, 0, 4, 0)\}, \quad \Delta_2(1) = \{(4, 0, 3, 1), (4, 1, 3, 0), (3, 1, 4, 0)\},$$
$$\Delta_2(2) = \{(4, 1, 2, 1), (3, 1, 3, 1), (3, 2, 3, 0)\}, \quad \Delta_2(3) = \{(3, 2, 2, 1)\}.$$

Theorem 1 *Let n be a positive integer. Then*

$$\sum_{r=-n}^{n} (-1)^r [(a^2b)^{n-r} \shuffle (a^2b)^{n+r}] = 3^n \sum_{k=0}^{2n-1} 2^{2n-k} \sum_{A(w)\in\Delta_n(k)} w.$$

In the following lemma, we show that Theorem 1 is equivalent to Conjecture 1, which is restated in terms of multiple zeta values. Using [4], we conclude that

$$\sum_{r=-n}^{n} (-1)^r \zeta(\{3\}^{n-r})\zeta(\{3\}^{n+r})$$
$$= 3^n \sum_{k=0}^{2n-1} 2^{2n-k} \sum_{(s_1, s_2 \dots, s_{2n})\in\Delta_n(k)} \zeta(s_1 + 1, s_2 + 1, \dots, s_{2n} + 1). \tag{12}$$

Lemma 1 *Let n and k be integers with $0 \le k < 2n$. Then*

$$\Xi_n(k) = \sum_{A(w)\in\Delta_n(k)} w.$$

Proof: Let $\bar{w} := (a^4b^2)^n$ and $A(\bar{w}) := (\bar{a}(1), \bar{a}(2), \dots, \bar{a}(2n))$, where $\bar{a}(1)$ is the number of times the letter a occurs to the left of b_1 in $\bar{w}$, and, for $1 < j \le |\bar{w}|_b$, $\bar{a}(j)$ is the number of times the letter a occurs between b_{j-1} and b_j, i.e.,

$$\bar{a}(j) = \begin{cases} 4, & \text{if } j \text{ is odd,} \\ 0, & \text{if } j \text{ is even.} \end{cases}$$

Note that $\bar{a}(w)$ satisfies (9).

We first show that for a given sequence $\pi \in \Delta_n(k)$, we can produce a word w from $\bar{w}$ using the allowed transpositions of a and b in $\bar{w}$. Let π be a sequence in $\Delta_n(k)$. We will make transpositions within $\bar{w}$ such that the number of a's on the left of b_1 becomes π_1 and the number of a's between b_{i-1} and b_i becomes π_j for $1 < i \le 2n$. Since π satisfies (9), $3 \le \pi_1 \le 4$ and $4 \le \pi_1 + \pi_2 \le 5$. There are four cases for (π_1, π_2): $(4, 0)$, $(4, 1)$, $(3, 1)$, and

$(3, 2)$. If $\pi_1 = 4$ and $\pi_2 = 0$, then we do not make any transposition of a single a in the first a^4 and a single b in the first b^2. If $\pi_1 = 4$ and $\pi_2 = 1$, then we transpose a single a among the second a^4 and a single b in the first b^2. If $\pi_1 = 3$ and $\pi_2 = 1$, then we transpose a single a among the first a^4 and single b in the first b^2. If $\pi_1 = 3$ and $\pi_2 = 2$, we transpose a single a in the first a^4 and a single b in the first b^2, and then transpose a single a in the second a^4 and the b which was not transposed in the first b^2. We make transpositions of single a's and single b's proceeding from the left in $\bar{w}$ in this way. Then we see that we can only use the allowed transpositions since π satisfies (9). Moreover, the number of transpositions we made is k since $\pi \in \Delta_n(k)$. Let w be the word with $A(w) = \pi$. Hence, w arises in $\Xi_n(k)$.

We now consider the reverse. In other words, we will show the $A(w)$ is in $\Delta_n(k)$ for a given w that arises in $\Xi_n(k)$. Since $\bar{a}(2i - 1) + \bar{a}(2i) = 4$ for $1 \le i \le n$, the transposition of a single a in the ith a^4 and a single b in the ith b^2 does not change $\bar{a}(2i - 1) + \bar{a}(2i) = 4$. If a transposition of a single a in the $(i + 1)$st a^4 and a single b in the ith b^2 is made, then $\bar{a}(2i - 1) + \bar{a}(2i)$ becomes 5. Suppose that w is a word arising in $\Xi_n(k)$. Since w is obtained from $\bar{w}$ by making k such transpositions, it can be easily shown that $A(w)$, the sequence of the number of a's between b's, satisfies (9). Furthermore, whenever a transposition is made, the number of the a's between the $(2i - 1)$st b and the $2i$th b increases by 1. Hence, $A(w) \in \Delta_n(k)$.   □

We now prove Theorem 1. In the alternating sum in this theorem, many words are cancelled because they appear with equal coefficients but opposite signs. We characterize the words cancelled in the alternating sum.

Lemma 2 *For a positive integer n and an integer r, $|r| \le n$, let w be a word in $S_{n,r}$ whose $A(w)$ does not belong to Δ_n. Then there is a unique r' with different parity from r such that the word w belongs to $S_{n,r'}$ as well. Furthermore, the number of occurrences of the word w in $S_{n,r}$ is equal to the number of occurrences in $S_{n,r'}$.*

Proof: Let m be the smallest positive integer for which (9) is not satisfied.

First, suppose that m is odd. Write $w = uv$, where u is the initial subword of w consisting of the letters from w_1 up to including b_m. Since $|u|_a = 2|u|_b = 2m$, we infer from Proposition 1 that there exists s with $s \le m$ and such that

$$u \in \{(a^2b)^s \, \shuffle \, (a^2b)^{m-s}\} \qquad \text{and} \qquad v \in \{(a^2b)^{n-r-s} \, \shuffle \, (a^2b)^{n+r-m+s}\}.$$

Since the shuffle product is commutative, $u' = u \in \{(a^2b)^{m-s} \, \shuffle \, (a^2b)^s\}$ as well. Let $w' := u'v$. Then $w' \in S_{n,r-m+2s}$. Since m is odd, the parity of $(r - m + 2s)$ must be opposite to the parity of r.

Now we show that the number of occurrences of the word w in $S_{n,r}$ and $S_{n,r-m+2s}$ are equal. Let $\sigma \in \text{Shuff}(n - r, n + r)$ be a shuffle corresponding to w. Then Proposition 1 implies that there exist shuffles τ and ρ corresponding to u and v, respectively.

We define a permutation τ' induced from τ by

$$\tau'(j) = \begin{cases} \tau(j) + 3m - 3s, & \text{if } 1 \le \tau(j) \le 3s, \\ \tau(j) - 3s, & \text{if } 3s + 1 \le \tau(j) \le 3m. \end{cases}$$

It is easily seen that τ' is a shuffle corresponding to u', and that τ' and ρ produce a unique shuffle σ' corresponding to w'.

On the other hand, suppose that m is even. Write $w = uv$, where u is the initial subword of w consisting of the letters from w_1 up to but excluding b_m. Proposition 1 now implies that there exists $s < m$ such that

$$u \in \{(a^2b)^s a^2 \amalg (a^2b)^{m-1-s} a^2\} \quad \text{and} \quad v \in \{b(a^2b)^{n-r-s-1} \amalg b(a^2b)^{n+r-m+s}\}.$$

Since the shuffle product is commutative, $u' = u \in \{(a^2b)^{m-1-s} a^2 \amalg (a^2b)^s a^2\}$ as well. Let $w' := u'v$. Then $w' \in S_{n,r-m+1+2s}$. Since m is even, the parity of $(r-m+1+2s)$ must be opposite to the parity of r.

As we did in the case when m is odd, we can show the number of occurrences of the word w in $S_{n,r}$ and $S_{n,r-m+1+2s}$ are equal. We omit the details. $\qquad\square$

Lemma 2 implies that there remain only the words w with $A(w) \in \Delta_n$ in the alternating sum in Theorem 1.

Proof of Theorem 1: Throughout this proof, we assume that any words arising from $\{u \amalg v\}$, $u, v \in \{a, b\}^*$, have negative and positive multiplicities if the difference of the numbers of b's in u and v is congruent to 2 and 0 modulo 4, respectively.

Let $Q_{n,r}$ be a multi-set consisting of those words in $S_{n,r}$ such that $A(w)$ belongs to Δ_n, and let Q_n be a hybrid set defined by

$$\{\cup_{r \text{ odd}} Q_{n,r} \mid \cup_{r \text{ even}} Q_{n,r}\}.$$

By the definition of S_n, Lemma 2, and the definition of Q_n, we can rewrite the alternating sum in Theorem 1 as

$$\sum_{|r| \leq n} (-1)^r \sum_{w \in S_{n,r}} w = \sum_{w \in S_n} w = \sum_{w \in Q_n} w.$$

Since Δ_n has the partition (11), to complete the proof of Theorem 1, it suffices to show that for each $0 \leq k < 2n$,

$$\sum_{w \in Q_n(k)} w = 3^n 2^{2n-k} \sum_{A(w) \in \Delta_n(k)} w, \tag{13}$$

where $Q_n(k)$ is a hybrid subset consisting of those words of Q_n such that $A(w)$ belongs to $\Delta_n(k)$.

To this end, let w be a word in $Q_n(k)$. Suppose that there are exactly $h = h(w)$ positive integers m that satisfy $\sum_{j=1}^m a(j) = 2m$, say, $m_1 < m_2 < \cdots < m_h = 2n$. Since w satisfies (9), m_p must be even for each $p = 1, 2, \ldots, h$. Let

$$u_1 := \prod_{j=1}^{3m_1} w_j, \qquad u_p := \prod_{j=3m_{p-1}+1}^{3m_p} w_j, \qquad 2 \leq p \leq h.$$

We call $w = u_1 u_2 \cdots u_h$ the *subword decomposition* of w, and write $m_p = m_p(w)$ when we want to emphasize the dependence of the sequence $m_1, m_2, \ldots$ on the word w.

It is necessary to partition $Q_n(k)$ into more refined hybrid subsets. Let α be a composition of n. In other words, α is a vector of positive integers whose components sum to n. Say $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_h) \in (\mathbb{Z}^+)^h$, where

$$|\alpha| := \sum_{j=1}^{h} \alpha_j = n.$$

For such α, let $Q_n^\alpha(k)$ be a hybrid set consisting of $w \in Q_n(k)$, where $m_p(w) = 2 \sum_{j=1}^{p} \alpha_j$ for $1 \leq p \leq h$. Then, by Definition 2,

$$Q_n^\alpha(k) = \dot{\bigcup_{|\tau|=k}} Q_{\alpha_1}^{(\alpha_1)}(\tau_1) \times \cdots \times Q_{\alpha_h}^{(\alpha_h)}(\tau_h), \tag{14}$$

where the union is over all compositions τ of k and the superscript (α_j) in $Q_{\alpha_j}^{(\alpha_j)}(\tau_j)$ is the composition of α_j with one part. By (14), the left hand side of the equality in (13) becomes

$$\sum_{w \in Q_n(k)} w = \sum_{|\alpha|=n} \sum_{w \in Q_n^\alpha(k)} w = \sum_{|\alpha|=n} \sum_{|\tau|=k} \prod_{j=1}^{h} \sum_{u_j \in Q_{\alpha_j}^{(\alpha_j)}(\tau_j)} u_j.$$

On the other hand, let $\Delta'_{\alpha_j}(\tau_j)$ be the subset of $\Delta_{\alpha_j}(\tau_j)$ such that $\sum_{l=1}^{m} \pi_l = 2m + 1$ for any even $m < 2\alpha_j$. Then subword decompositions imply that

$$\sum_{A(w) \in \Delta_n(k)} w = \sum_{|\alpha|=n} \sum_{|\tau|=k} \prod_{j=1}^{h} \sum_{A(u_j) \in \Delta'_{\alpha_j}(\tau_j)} u_j.$$

Hence, it suffices to prove that

$$\sum_{w \in Q_n^{(n)}(k)} w = 3^n 2^{2n-k} \sum_{A(w) \in \Delta'_n(k)} w. \tag{15}$$

Recall that $|w|_b = 2n$ and $a(2) + a(4) + \cdots + a(2n) = k$. We write w as $s_1 \cdots s_n$, where s_1 contains the letters from the leftmost letter of w up to including b_2, and s_j contains the letters from the letter immediately following $b_{2(j-1)}$ up to including b_{2j} for $j > 1$. Note that any distinct word w in Q_n is determined by the sequence $a(i)$ for $1 \leq i \leq 2n$ from the

definition of Q_n. We rewrite the conditions for the sequence π, where $\pi \in \Delta'_n(k)$, as

$$
\begin{cases}
2m + 1 \leq \displaystyle\sum_{j=1}^{m} \pi_j \leq 2m + 2, & \text{if } m \text{ is odd,} \\[2ex]
\displaystyle\sum_{j=1}^{m} \pi_j = 2m + 1, & \text{if } m \neq 2n \text{ is even,} \\[2ex]
\displaystyle\sum_{j=1}^{m} \pi_j = 2m, & \text{if } m = 2n, \\[1ex]
\pi_2 + \pi_4 + \cdots + \pi_{2n} = k.
\end{cases}
\tag{16}
$$

We will count the number of $w \in Q_n^{(n)}(k)$ in (15) with $A(w) = \pi$ for a given sequence $\pi \in \Delta'_n(k)$.

Let $n = 1$. Then $\pi_1 + \pi_2 = 4$. From (16), $3 \leq \pi_1 \leq 4$, and $0 \leq \pi_2 \leq 1$. Thus $w \in \{|(a^2b) \shuffle (a^2b)\}$. Now, we count the multiplicity of w in $\{|(a^2b) \shuffle (a^2b)\}$. If $\pi_1 = 4$, then $w = a^4bb$. Otherwise, $w = a^3bab$. If $w = a^4bb$, then there are $3 \cdot 2^2$ w in $(a^2b) \shuffle (a^2b)$. Otherwise, there are only $3 \cdot 2$ w from the shuffle rule. Hence, there are $3^n \cdot 2^{2n-e(\pi)}$ w in (15), and w comes from $\{|(a^2b) \shuffle (a^2b)\}$.

Let $n \geq 2$. From (16), $\pi_1 + \pi_2 = 5$ and $\pi_{2n-1} + \pi_{2n} = 3$. We decompose w into $s_1 \cdots s_n$ and first examine s_1. There are two cases: $\pi_1 = 4, \pi_2 = 1$ and $\pi_1 = 3, \pi_2 = 2$. In other words, s_1 is either a^4bab or a^3ba^2b. Thus s_1 comes from one of the hybrid sets

$$A_1 = \{a \shuffle (a^2b)^2 \,|\, (a^2b)a \shuffle (a^2b)\}$$

or

$$A_2 = \{(a^2b)^2 \shuffle a \,|\, (a^2b) \shuffle (a^2b)a\}.$$

If s_1 is a^4bab, then it appears on the right of the bars in A_1 and A_2; s_1 occurs in A_1 with multiplicity $6 = 3 \cdot 2^{2-\pi_2}$ by (2). By symmetry, $s_1 = a^4bab$ occurs in A_2 with multiplicity 6. On the other hand, if s_1 is a^3ba^2b, then it appears on both sides in A_1 and A_2. Using (2), we easily find that s_1 occurs with multiplicity 3 on the left sides and multiplicity $3 \cdot 2$ on the right sides in A_1 and A_2. Thus the multiplicity of s_1 becomes $3 = 3 \cdot 2^{2-\pi_2}$ in A_1 and A_2 after cancellation.

Similarly, s_n is either a^3bb or a^2bab, which come from one of the hybrid sets

$$C_1 = \{ab \shuffle a^2b\} \qquad \text{or} \qquad C_2 = \{a^2b \shuffle ab\}.$$

Either of these multi-sets contains $s_n = a^3bb$ with multiplicity $6 = 3 \cdot 2^{1-\pi_{2n}}$ and $s_n = a^2bab$ with multiplicity $3 = 3 \cdot 2^{1-\pi_{2n}}$.

If $n = 2$, then any $w \in Q_n^{(n)}$ comes from the hybrid set

$$A_1 \times C_1 \cup A_2 \times C_2,$$

and so its multiplicity in $Q_n^{(n)}$ is

$$3 \cdot 2^{2-\pi_2} \cdot 3 \cdot 2^{1-\pi_4} + 3 \cdot 2^{2-\pi_2} \cdot 3 \cdot 2^{1-\pi_4} = 3^2 \cdot 2^{4-\pi_2-\pi_4} = 3^2 \cdot 2^{4-e(\pi)}.$$

For the cases when $n \geq 3$, we must consider s_i with $1 < i < n$. From (16), we see that $\pi_{2i-1} + \pi_{2i} = 4$. Thus s_i is either a^3bab or a^2ba^2b, which come from one of the four hybrid sets

$$B_{11} = \{1 \sqcup\!\sqcup (a^2b)^2 \,|\, aba \sqcup\!\sqcup a^2b\},$$
$$B_{12} = \{ab(a^2b) \sqcup\!\sqcup a \,|\, ab \sqcup\!\sqcup (a^2b)a\},$$
$$B_{21} = \{a \sqcup\!\sqcup ab(a^2b) \,|\, (a^2b)a \sqcup\!\sqcup ab\},$$
$$B_{22} = \{(a^2b)^2 \sqcup\!\sqcup 1 \,|\, a^2b \sqcup\!\sqcup aba\}.$$

If $s_i = a^3bab$, then it cannot appear on the left sides of the bars in the four hybrid sets above. The multiplicity of $s_i = a^3bab$ is $3 = 3 \cdot 2^{1-\pi_{2i}}$ in each of these hybrid sets, while that of a^2ba^2b is 3 in B_{11} and B_{22}, and 0 in B_{12} and B_{21} after cancellation, since $s_i = a^2ba^2b$ occurs with multiplicity 1 on the left of the bar and with multiplicity 4 on the right of the bar in B_{11}, and it occurs with multiplicity 1 on both sides in B_{12}. Then, for example, any $w \in Q_4^{(4)}$ comes from the hybrid set

$$A_1 \times B_{11} \times B_{11} \times C_1 \cup A_1 \times B_{11} \times B_{12} \times C_2 \cup A_1 \times B_{12} \times B_{21} \times C_1 \cup A_1 \times B_{12}$$
$$\times B_{22} \times C_2 \cup A_2 \times B_{21} \times B_{11} \times C_1 \cup A_2 \times B_{21} \times B_{12} \times C_2 \cup A_2 \times B_{22} \times B_{21}$$
$$\times C_1 \cup A_2 \times B_{22} \times B_{22} \times C_2,$$

with each of the B_{ij} occurring in each position exactly one fourth of the time. In general, any $w \in Q_n^{(n)}$ comes from the hybrid set

$$\bigcup_I A_{i_1} \left(\prod_{j=2}^{n-1} B_{i_{j-1}i_j} \right) C_{i_{n-1}},$$

where I runs over all distinct sequences $(i_1, \ldots, i_{n-1})$ consisting of 1's and 2's. Each of the B_{ij} occurs in each position exactly one fourth of the time. We see that the average multiplicity of $s_i = a^3bab$ is $3 = 3 \cdot 2^{1-\pi_{2i}}$, and of $s_i = a^2ba^2b$ is $3/2 = 3 \cdot 2^{1-\pi_{2i}}$. Since the decomposition of $Q_n^{(n)}$ has 2^{n-1} terms, the total multiplicity of $w = s_1 \cdots s_n = a^{\pi_1}ba^{\pi_2}b \cdots a^{\pi_{2n-1}}ba^{\pi_{2n}}b$ in $Q_n^{(n)}$ is

$$2^{n-1} \cdot 3 \cdot 2^{2-\pi_2} \prod_{i=2}^{n-1}(3 \cdot 2^{1-\pi_{2i}}) \cdot 3 \cdot 2^{1-\pi_{2n}} = 3^n \cdot 2^{2n-e(\pi)},$$

which completes the proof. $\square$

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