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Some Multi-Set Inclusions Associated with Shuffle Convolutions and Multiple Zeta Values

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Abstract. We outline a new technique for proving certain shuffle convolution formulæ. As an application, we give a new combinatorial proof of the formula $\zeta(\{3,1\}^n) = 2\pi^{4n}/(4n+2)!$ for multiple zeta values.

1 Shuffles

As in [5, 6, 13] let X be a finite set and let X^* denote the free monoid generated by X. We regard X as an alphabet, and the elements of X^* as words formed by concatenating any finite number of letters (repetitions permitted) from the alphabet X. By linearly extending the concatenation product to the set $\mathbf{Q}\langle X\rangle$ of rational linear combinations of elements of X^*, we obtain a non-commutative polynomial ring with the elements of X being indeterminates and with multiplicative identity 1 denoting the empty word.

The shuffle product may be defined on words by the recursion

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

and then extended linearly to $\mathbf{Q}\langle X\rangle$. One checks that the shuffle product so defined is associative and commutative, and thus $\mathbf{Q}\langle X\rangle$ equipped with the shuffle product becomes a commutative $\mathbf{Q}$-algebra, denoted $\mathrm{Sh}_{\mathbf{Q}}[X]$. Radford [14] has shown that $\mathrm{Sh}_{\mathbf{Q}}[X]$ is isomorphic to the polynomial algebra $\mathbf{Q}[L]$ obtained by adjoining the transcendence basis L of Lyndon words to the field $\mathbf{Q}$ of rational numbers. The study of shuffles was initiated by Chen [8, 9] and subsequently formalized by Ree [15]. Interest in shuffles has revived due to the intimate connection with multiple zeta values [1, 3, 4, 5, 7, 11, 12, 16] and multiple polylogarithms [2, 6, 10, 17].

In what follows, if X is an alphabet and $u, v \in X^*$, we'll denote by $\{u \sqcup\!\sqcup\, v\}$ the multi-set of words appearing (with multiplicity) in the expansion of $u \sqcup\!\sqcup\, v$. For example, suppose $X = \{a, b\}$. Since $ab \sqcup\!\sqcup\, ab = 4aabb + 2abab$, we have

$$\{ab \sqcup\!\sqcup\, ab\} = \{abab, abab, aabb, aabb, aabb, aabb\},$$

which, as a multi-set, *properly* contains $\{abab, aabb\}$.

Theorem 1 *Let r be a positive integer, let X be an alphabet, and let $a_1, a_2, \ldots \in X$ be such that $a_{r+k} = a_k$ for all positive integers k. Fix a positive integer n, and define multi-sets*

$$S_k = \{a_1a_2 \cdots a_{kr} \sqcup\!\sqcup\, a_1a_2 \cdots a_{(2n-k)r}\}, \qquad 0 \le k \le 2n.$$

Then $S_{k-1} \subseteq S_k$ for $k = 1, 2, \ldots, n$, and $S_{k+1} \subseteq S_k$ for $k = n, n+1, \ldots, 2n-1$.

2 Consequences

Before proving Theorem 1, we make some observations. First, observe that Theorem 1 generalizes the unimodality of the binomial coefficients. More specifically, we have the following:

Corollary 1 *Let n and r be positive integers. The finite sequence $b_0, b_1, \ldots, b_{2n}$ defined by*

$$b_k = \binom{2nr}{kr}, \qquad 0 \le k \le 2n,$$

is unimodal.

Proof. Note that the cardinality of the multi-set S_k in Theorem 1 is equal to b_k. □

More interestingly, Theorem 1 implies a non-trivial shuffle convolution formula which has been shown [3] to imply the formula

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

for the multiple zeta function defined by

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

Corollary 2 *Let n be a positive integer, and let $\{a,b\}$ be an alphabet. Then*

$$\sum_{k=0}^{2n} (-1)^{n+k} [(ab)^k \sqcup\!\sqcup\, (ab)^{2n-k}] = (4a^2b^2)^n. \tag{2}$$

Proof. In Theorem 1, let $X = \{a,b\}$ and $r = 2$. In view of the multi-set inclusions indicated by Theorem 1, there must be

$$\sum_{k=0}^{2n} (-1)^{n+k} |S_k| = \sum_{k=0}^{2n} (-1)^{n+k} \binom{4n}{2k} = 4^n$$

terms on each side of (2), counting multiplicity. Furthermore, the word $(a^2b^2)^n$ occurs 4^n times in S_n, since each a and each b can take two positions. Since $(a^2b^2)^n$ cannot occur in S_k for $k \neq n$, (2) follows immediately. □

Corollary 3 *The formula (1) holds, i.e. if n is a positive integer, then*

$$\zeta(\{3,1\}^n) = \frac{2\pi^{4n}}{(4n+2)!}.$$

Proof. The stated formula follows from (2) and the iterated integral representation for multiple zeta values. See [3] for details. □

3 Proving the Multi-Set Inclusions

Proof of Theorem 1. Since $S_k = S_{2n-k}$, it suffices to prove that $S_{k-1} \subseteq S_k$ for $k = 1, 2, \ldots, n$. We shall first consider the case when $k = 1$. Observe that

$$S_1 = \{a_1 \cdots a_r \sqcup\!\sqcup\, a_1 \cdots a_{(2n-1)r}\}$$

and that $S_0 = \{a_1 a_2 \cdots a_{2nr}\}$. Since periodicity implies

$$a_1 \cdots a_{2nr} = a_1 \cdots a_r a_{r+1} \cdots a_{2nr} = a_1 \cdots a_r a_1 \cdots a_{(2n-1)r} \in S_1$$

it follows that $S_0 \subseteq S_1$, and so we may assume henceforth that $2 \le k \le n$.

To help clarify the formation of words in the multi-sets S_k, for $0 \le k \le n$, let

$$S_k = \{a_1 \cdots a_{kr} \sqcup\!\sqcup A_1 \cdots A_{(2n-k)r}\},$$

where $A_j = a_j$ for each positive integer j. Now consider a word

$$w \in S_{k-1} = \{a_1 \cdots a_{(k-1)r} \sqcup\!\sqcup A_1 \cdots A_{(2n-k+1)r}\}.$$

If a_1 follows A_r in w, then

$$\begin{aligned} w &\in A_1 \cdots A_r\{a_1 \cdots a_{(k-1)r} \sqcup\!\sqcup A_{r+1} \cdots A_{(2n-k+1)r}\} \\ &= a_1 \cdots a_r\{a_{r+1} \cdots a_{kr} \sqcup\!\sqcup A_1 \cdots A_{(2n-k)r}\} \\ &\subseteq S_k. \end{aligned}$$

Since we could conceivably have made a different choice in replacing certain of the A_j by a_j, it follows that the multiplicity of w in S_k is no less than the multiplicity of w in S_{k-1} in this case. Therefore, we may assume a_1 precedes A_r in w. If, in addition, a_2 follows A_{r+1} in w, then

$$\begin{aligned} w &\in \{A_1 \cdots A_{r-1} \sqcup\!\sqcup a_1\}A_r A_{r+1}\{a_2 \cdots a_{(k-1)r} \sqcup\!\sqcup A_{r+2} \cdots A_{(2n-k+1)r}\} \\ &= \{a_1 \cdots a_{r-1} \sqcup\!\sqcup A_1\}a_r a_{r+1}\{a_{r+2} \cdots a_{kr} \sqcup\!\sqcup A_2 \cdots A_{(2n-k)r}\} \\ &\subseteq S_k. \end{aligned}$$

Therefore, we may assume a_2 precedes A_{r+1} in w.

In general, given that a_p precedes A_{r+p-1} in w, we note that if a_{p+1} follows A_{r+p}, then w lies in the multi-set

$$\begin{aligned} &\{A_1 \cdots A_{r+p-2} \sqcup\!\sqcup a_1 \cdots a_p\}A_{r+p-1}A_{r+p}\{a_{p+1} \cdots a_{(k-1)r} \sqcup\!\sqcup A_{r+p+1} \cdots A_{(2n-k+1)r}\} \\ = &\{a_1 \cdots a_{r+p-2} \sqcup\!\sqcup A_1 \cdots A_p\}a_{r+p-1}a_{r+p}\{a_{r+p+1} \cdots a_{kr} \sqcup\!\sqcup A_{p+1} \cdots A_{(2n-k)r}\} \\ \subseteq &S_k. \end{aligned}$$

By induction, we may therefore assume that $a_{(k-1)r}$ precedes A_{kr-1} in w, in which case w must lie in the multi-set

$$\begin{aligned} &\{a_1 \cdots a_{(k-1)r} \sqcup\!\sqcup A_1 \cdots A_{kr-2}\}A_{kr-1} \cdots A_{(2n-k+1)r} \\ = &\{A_1 \cdots A_{(k-1)r} \sqcup\!\sqcup a_1 \cdots a_{kr-2}\}a_{kr-1}a_{kr}A_{kr+1} \cdots A_{(2n-k+1)r} \\ = &\{A_1 \cdots A_{(k-1)r} \sqcup\!\sqcup a_1 \cdots a_{kr-2}\}a_{kr-1}a_{kr}A_{(k-1)r+1} \cdots A_{(2n-k)r} \\ \subseteq &S_k. \end{aligned}$$

□

Other shuffle convolution formulæ can be established in a similar manner. For example, if $\{a, b\}$ is an alphabet and n is a positive integer, then

$$2\sum_{k=0}^{2n}(-1)^{n+k}[(ab)^k \sqcup\!\sqcup (ba)^{2n-k}] = (4abba)^n + (4baab)^n.$$

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