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Identities for the Multiple Polylogarithm Using the Shuffle Operation

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IDENTITIES FOR THE MULTIPLE POLYLOGARITHM USING THE SHUFFLE OPERATION

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At the beginning of my research, I understood the shuffle operation and iterated integrals to make a new proof-method (called a combinatorial method). As a first work, I proved an combinatorial identity 2 using a combinatorial method. While proving it, I got four identities and showed that one of them is equal to an analytic identity 1 which is found at the paper [2] written by David M. Bradley and Doug Bowman. Furthermore, I derived an formula involving nested harmonic sums. Using Maple (a mathematical software), I found a new combinatorial identity 3 and derived two formulas: One is related to multiple polylogarithms and the other is related to rational functions. Since letters in the identities represent differential 1-forms which converge, I can find new formulas if I get a proper setting.

My research was developed by considering a combinatorial identity 4 given by David M. Bradley, thesis advisor. Though it looked very complicated, the implication for the identity was very interesting to me. Using a combinatorial proof-method, I proved it. Even though I just derived one formula involving nested harmonic sums in this thesis, the identity has potentiality because, if I find a new setting for differential 1-forms, I can derive a new formula involving multiple polylogarithms.

It was not very easy to prove the combinatorial identity 4 even though I used the combinatorial proof-method as I did at the proofs of the combinatorial identity 2 and 3. The reason is that the result of the identity 4 is more complicated than those of the identities 3 and 4. So, Lemma 5 is needed to complete the proof of the identity 4, which step is not needed in the proofs of the identities 3 and 4. When formulating the identity 4, I had a trouble in defining the notations because of their complexity. When I formulated the identity 4, it was a beautiful formula

As we can see in the paper [3], there are various conjectures related to multiple zeta values whose incompletion is a sign that both the mathematics and physics communities do not yet completely understand the field. At this situation, this combinatorial proof-method can play a crucial role in developing other fields such as knot theory and quantum field theory as well as combinatorics.

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Chapter 1

INTRODUCTION

1.1 The Riemann zeta function.

The Riemann zeta function is the function of the complex variable s, defined in the half-plane $Re(s) > 1$ by the absolutely convergent series

$$\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s},$$

and in the whole complex plane $\mathbf{C}$ by analytic continuation. As shown by Riemann, $\zeta(s)$ extends to $\mathbf{C}$ as a meromorphic function with only a simple pole at $s = 1$, with residue 1, and satisfies the functional equation

$$\pi^{-\frac{s}{2}}\Gamma(\frac{s}{2})\zeta(s) = \pi^{-\frac{1-s}{2}}\Gamma(\frac{1-s}{2})\zeta(1-s).$$

1.2 Multiple zeta functions.

We generalize the Riemann zeta function to the multiple zeta functions in the following way:

The multiple zeta functions are defined by

$$\zeta(s_1, \cdots, s_k) := \sum_{n_1 > n_2 > \cdots > n_k > 0} \prod_{j=1}^{k} \frac{1}{n_j^{s_j}},$$

where $s_j \in \mathbf{C}, Re(s_1) > 1$ and $\sum_{j=1}^{k} Re(s_j) > k$.

Jiangiang Zhao's paper[1] shows that the multiple zeta function can be analytically continued to a meromorphic function on all of **C**. But there still exist two open problems:

1. Determine the complete set of trivial (resp. nontrivial) zeros of the multiple zeta function.

2. Determine the functional equation (if any) of the multiple zeta functions which generalize the classical functional equation of the Riemann zeta function.

1.3 Nested harmonic sums.

Let $\omega_1, \cdots, \omega_n$ be complex-valued differential 1-forms defined on a real interval $[a,b]$. We have $\omega_i = f_i(s)ds$ where $f_1, \cdots, f_n$ are complex functions. Define the iterated integral $\int_a^b \omega_1 \cdots \omega_n$ inductively by

$$\int_a^b \omega_1 = \int_a^b f_1(s)ds$$

and

$$\int_a^b \omega_1 \cdots \omega_n = \int_a^b f_1(s)(\int_a^s \omega_2 \cdots \omega_n ds) \; if \; n > 1.$$

Nested harmonic sums of arbitrary depth k (or k-fold Euler sums) and their $(s_1 + s_2 + \cdots + s_k)$-dimensional iterated integral representations are defined by

$$\begin{aligned} \zeta(s_1, \cdots, s_k; a_1, \cdots, a_k) &= \sum_{n_1 > n_2 > \cdots > n_k > 0} \prod_{j=1}^{k} \frac{a_j^{n_j}}{n_j^{s_j}} \\ &\quad where \; a_j = \pm 1 \; and \; s_1 a_1 \neq 1 \\ &= \int_0^1 \Omega^{s_1 - 1}\omega_1 \cdots \Omega^{s_k - 1}\omega_k \\ &\quad where \; \Omega = \frac{dx}{x}, \omega_j = \frac{\tau_j dx_j}{1 - \tau_j x_j}, \tau_j = \prod_{i=1}^{j} a_i \\ &\quad and \; s_j \; are \; positive \; integers. \end{aligned}$$

Example 1.3.1.

$$\begin{aligned}\zeta(2,1;-1,1) &= \sum_{n_1>n_2>0} \frac{(-1)^{n_1}}{n_1^2 n_2} \\ &= \int_0^1 \frac{dx_1}{x_1} \int_0^{x_1} \frac{-dx_2}{1+x_2} \int_0^{x_2} \frac{-dx_3}{1+x_3}.\end{aligned}$$

1.4 The multiple polylogarithm.

We define the multiple polylogarithm by

$$\zeta(s_1,\cdots,s_k;a_1,\cdots,a_k) = \sum_{n_1>n_2>\cdots>n_k>0} \prod_{j=1}^{k} \frac{a_j^{n_j}}{n_j^{s_j}},$$

where s_j and $a_j \in \mathbf{C}$.

The multiple polylogarithm is the extension of the nested harmonic sums and the multiple zeta functions because they extend the variables s_j and a_j of nested harmonic sums to any complex numbers and let us control the increasing and decreasing speed of the multiple zeta functions by the each a_j as n_j is increasing. For example, the decreasing speed of values $\zeta(2;\frac{1}{2})$ is faster than that of $\zeta(2;1)$ as n is increasing.

1.5 The shuffle operation.

Let $\mathcal{A}$ denote a finite set of letters; let $\mathcal{A}^*$ denote the set of all words on $\mathcal{A}$. Define $\sqcup$ (Shuffle operation) by $u \sqcup v = \sum x_{\sigma(1)}x_{\sigma(2)}\cdots x_{\sigma(n+m)}$, for $u = x_1\cdots x_n \in \mathcal{A}^*$ and $v = x_{n+1}\cdots x_{n+m} \in \mathcal{A}^*$, where the sum is over all $\binom{n+m}{n}$ permutations σ of the set $\{1,2,\cdots,n+m\}$ which satisfy $\sigma^{-1}(j) < \sigma^{-1}(k)$ for all $1 \le j < k \le n$ and $n+1 \le j < k \le n+m$.

Example 1.5.1.

$$abb \sqcup ab = 6a^2b^3 + 3abab^2 + ab^2ab.$$

The shuffle operation $\sqcup$ can be extended linearly to the non-commutative polynomial ring $\mathbf{Q} < \mathcal{A} >$ in the natural way. This makes $\mathbf{Q} < \mathcal{A} >$ into a commutative associative $\mathbf{Q}$-algebra with multiplication $\sqcup$.

Example 1.5.2.

$$ab \sqcup (3ba - 2ab) = 6ab^2a - abab + 3baba + 6ba^2b - 8a^2b^2.$$

Iterated integrals satisfy the following property: Let $\omega_1, \cdots, \omega_{n+m}$ be complex-valued differential 1-forms defined on a real interval $[a, b]$, then

$$\int_a^b \omega_1 \cdots \omega_n \int_a^b \omega_{n+1} \cdots \omega_{n+m} = \sum_\sigma \int_a^b \omega_{\sigma_1} \cdots \omega_{\sigma_{n+m}},$$

where σ runs over all (n, m)-shuffles of the symmetric group S_{n+m}, which shows that the product of nested harmonic sums can be decomposed using the shuffle operation.

Example 1.5.3.

$$\begin{aligned}
\zeta(2,1;1,1)\zeta(2;1) &= \int_0^1 \Omega\omega\omega \int_0^1 \Omega\omega \textit{ where } \omega = \frac{dx}{1-x} \\
&= 6\int_0^1 \Omega^2\omega^3 + 3\int_0^1 \Omega\omega\Omega\omega^2 + \int_0^1 \Omega\omega^2\Omega\omega \\
&= 6\zeta(3,1,1;1,1,1) + 3\zeta(2,2,1;1,1,1) \\
&+ \zeta(2,1,2;1,1,1)
\end{aligned}$$

1.6 The multi-set.

We define a multi-set by a collection whose repeated elements are allowed. So the multi-set $\{a, b, c, c\}$ is the same as the multi-set $\{a, b, 2c\}$ but distinct from the multi-set $\{a, b, c\}$. Contrast this with the set $\{a, b, c, c\}$ which is the same as the set $\{a, b, c\}$.

The number of repetitions of each member is called the *multiplicity* of that member. For the multi-set $\{a, b, c, c\}$, the multiplicity of a and b is 1, and the multiplicity of c is 2.

Let A and B be multi-sets, we define $A = B$ to mean that every element of A is an element of B, their multiplicities are equal and vice versa. We also define $A \subset B$ to mean that every element of A is an element of B and the multiplicity of each element of A is less than or equal to that of B. If $A \subset B$ and $A \neq B$, we say that A is a strict multi-subset(or subset) of B.

Example 1.6.1. Let S be the multi-set of all words as the result of $ab^2 \sqcup ab$. Then

$$\begin{aligned} S &= \{a^2b^3, a^2b^3, a^2b^3, a^2b^3, a^2b^3, a^2b^3, abab^2, abab^2, abab^2, ab^2ab\} \\ &= \{6a^2b^3, 3abab^2, ab^2ab\}. \end{aligned}$$

Furthermore, $\{a^2b^3, abab^2, ab^2ab\}$ is a strict multi-subset of S.

Chapter 2

IDENTITIES FOR MULTIPLE POLYLOGARITHMS

2.1 Analytic identity 1 and its formula for nested harmonic sums.

Proposition 1 .

$$\sum_{n\geq 0}(-1)^n z^{4n}\int_0^x (4a^2b^2)^n = \sum_{k\geq 0}(-1)^k z^{2k}\int_0^x (ab)^k \sum_{m\geq 0} z^{2m}\int_0^x (ab)^m$$

where a and b are any differential forms whose integrals converge.

Proof. Let $a = f(x)dx$ and $b = g(x)dx$; let $D_a = \frac{1}{f(x)}\frac{d}{dx}$ and $D_b = \frac{1}{g(x)}\frac{d}{dx}$; let $F(x,z) := \sum_{n\geq 0}(-1)^n z^{4n}\int_0^x (4a^2b^2)^n$, then

$$\begin{aligned} D_aF(x,z) &= \frac{1}{f(x)}\frac{d}{dx}\sum_{n\geq 0}(-1)^n z^{4n}\int_0^x 4^n a^2b^2(a^2b^2)^{n-1} \\ &= \sum_{n\geq 0}(-1)^n 4^n z^{4n}\frac{1}{f(x)}\frac{d}{dx}\int_0^x a^2b^2(a^2b^2)^{n-1} \\ &= \sum_{n\geq 0}(-1)^n 4^n z^{4n}\int_0^x ab^2(a^2b^2)^{n-1} \end{aligned}$$

Taking D_a^2F, $D_bD_a^2F$, and $D_b^2D_a^2F$ in this order on both sides, we obtain

$$\begin{aligned} D_b^2D_a^2F(x,z) &= \sum_{n\geq 0}(-1)^{n+1}z^{4n+4}4^{n+1}\int_0^x (a^2b^2)^n \\ &= -4z^4F(x,z). \end{aligned}$$

So, $F(x,z)$ is a solution of 4th order differential equation $D_b^2D_a^2 + 4z^4 = 0$.

Let $G(x,z) := \sum_{k\geq 0}(-1)^k z^{2k}\int_0^x (ab)^k \sum_{m\geq 0} z^{2m}\int_0^x (ab)^m$, then

$$\begin{aligned} D_a G(x,z) &= \sum_{k\geq 1}(-1)^k z^{2k}\int_0^x b(ab)^{k-1}\sum_{m\geq 0} z^{2m}\int_0^x (ab)^m \\ &+ \sum_{k\geq 0}(-1)^k z^{2k}\int_0^x (ab)^k\sum_{m\geq 1} z^{2m}\int_0^x b(ab)^{m-1} \\ &= \sum_{k\geq 0}(-1)^{k+1} z^{2k+2}\int_0^x b(ab)^k\sum_{m\geq 0} z^{2m}\int_0^x (ab)^m \\ &+ \sum_{k\geq 0}(-1)^k z^{2k}\int_0^x (ab)^k\sum_{m\geq 0} z^{2m+2}\int_0^x b(ab)^m \end{aligned}$$

Taking $D_a^2 G$, $D_b D_a^2 G$, and $D_b^2 D_a^2 G$ in this order on both sides, we obtain

$$D_b^2 D_a^2 G(x,z) = -4z^4 G(x,z)$$

So, $G(x,z)$ is also a solution of $D_b^2 D_a^2 + 4z^4 = 0$.

We can get four initial conditions, putting $x = 0$ at the each step taking D_a, D_a^2, $D_b D_a^2$, and $D_b^2 D_a^2$ on both sides: $F(0,z) = G(0,z)$, $D_a F(0,z) = D_a G(0,z)$, $D_a^2 F(0,z) = D_a^2 G(0,z)$ and $D_b D_a^2 F(0,z) = D_b D_a^2 G(0,z)$, Then $F(x,z) = G(x,z)$.

In Proposition 1, if we take $a = \frac{dx}{x}$ and $b = \frac{dx}{1-x}$, then we can get the following formula involving nested harmonic sums:

Formula 2 .

$$\sum_{n\geq 0}(-1)^n z^{4n}\zeta(\{3,1\}^n;\{1,1\}^n) = \sum_{k\geq 0}(-1)^k z^{2k}\zeta(\{2\}^k;\{1\}^k)\sum_{m\geq 0} z^{2m}\zeta(\{2\}^m;\{1\}^m),$$

where the notation $\{X\}^n$ *indicates* n *successive instances of the integer sequence* X.

Proof. Let $a = \frac{dx}{x}$ and $b = \frac{dx}{1-x}$. Apply a and b to Proposition 1, then we have the followings:

$$
\begin{aligned}
L.H.S &= \sum_{n\geq 0}(-1)^n z^{4n}\int_0^1 (4a^2b^2)^n \\
&= \sum_{n\geq 0}(-1)^n z^{4n}4^n\zeta(\{3,1\}^n;\{1,1\}^n)
\end{aligned}
$$

and

$$
\begin{aligned}
R.H.S &= \sum_{k\geq 0}(-1)^k z^{2k}\int_0^1 (ab)^k \sum_{m\geq 0} z^{2m}\int_0^1 (ab)^m \\
&= \sum_{k\geq 0}(-1)^k z^{2k}\zeta(\{2\}^k;\{1\}^k)\sum_{m\geq 0} z^{2m}\zeta(\{2\}^m;\{1\}^m).
\end{aligned}
$$

Hence we have the following formula:

$$
\begin{aligned}
L.H.S &= \sum_{n\geq 0}(-1)^n z^{4n}\zeta(\{3,1\}^n;\{1,1\}^n) \\
&= \sum_{k\geq 0}(-1)^k z^{2k}\zeta(\{2\}^k;\{1\}^k)\sum_{m\geq 0} z^{2m}\zeta(\{2\}^m;\{1\}^m) \\
&= R.H.S.
\end{aligned}
$$

2.2 Combinatorial identity 2 for nested harmonic sums.

Theorem 3 .

$$
\begin{aligned}
& \{1+(\frac{t}{1-i})a+(\frac{t}{1-i})^2ab+(\frac{t}{1-i})^3aba+(\frac{t}{1-i})^4abab+\cdots\} \\
\sqcup\ & \{1+(\frac{t}{1+i})a+(\frac{t}{1+i})^2ab+(\frac{t}{1+i})^3aba+(\frac{t}{1+i})^4abab+\cdots\} \\
=\ & 1+ta+t^2a^2+t^3a^2b+t^4a^2b^2+t^5a^2b^2a+t^6a^2b^2a^2+\cdots
\end{aligned}
$$

where $t \in \mathbf{C}$.

Proof. In the following lemmas we show that the coefficients of t^{4n}, t^{4n+1}, t^{4n+2} and t^{4n+3} for $n \in \mathbf{N}$ in the two series given in Theorem 3 coincide. This will establish the proof of Theorem 3. Afterwards, we can obtain four identities involving multiple polylogarithms as formulas to the four lemmas if we find a proper setting of a and b.

2.2.1 The coefficient of t^{4n}.

Let us find the coefficient of t^{4n} in the left hand side in Theorem 3 and show the equality between the coefficients on both sides:

Lemma 1 . *The coefficient of t^{4n} in Theorem 3 is:*

$$\frac{1}{4^n}\sum_{|r|\le n}(-1)^r[(ab)^{n-r}\sqcup(ab)^{n+r}]=(a^2b^2)^n.$$

Proof. Let us investigate first several terms on the left hand side to find the pattern:

$$\begin{aligned}&(\frac{t}{1+i})^4abab+(\frac{t}{1-i})(\frac{t}{1+i})^3(a\sqcup aba)+(\frac{t}{1-i})^2(\frac{t}{1+i})^2(ab\sqcup ab)\\+\ &(\frac{t}{1-i})^3(\frac{t}{1+i})(aba\sqcup a)+(\frac{t}{1-i})^4abab+\cdots.\end{aligned}$$

The shuffle operation is commutative and we have the following computations: $(\frac{1}{1-i})^4=(\frac{1}{1+i})^4=-\frac{1}{4}$, $(\frac{1}{1-i})^3(\frac{1}{1+i})^1=\frac{i}{4}$, $(\frac{1}{1-i})^2(\frac{1}{1+i})^2=\frac{1}{4}$, and $(\frac{1}{1-i})^1(\frac{1}{1+i})^3=-\frac{i}{4}$. Therefore we obtain the coefficient of t^{4n} on the left hand side as

$$\frac{1}{4^n}\sum_{|r|\le n}(-1)^r[(ab)^{n-r}\sqcup(ab)^{n+r}].$$

Putting $k=n-r$, we can rewrite the statement of the lemma as the following:

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

We will prove this statement.

Let S_k be the multi-set of all words as the result of $(ab)^k \sqcup (ab)^{2n-k}$, for $0 \leq k \leq n$. Then we get the following inclusion by Lemma 6 [Inclusion of multi-set 1]: S_k for $0 \leq k \leq 2n$ and $k \neq n$. Since the shuffle operation is commutative, then $S_{2n-k} = S_k$. Hence every word on the left hand side is contained in S_n.

On the other hand, we know that $(a^2b^2)^n$ is not contained in S_k for $0 \leq k \leq 2n$ and $k \neq n$. Consider the formation of $(a^2b^2)^n$ in detail. If we let $(ab)^n$ be $(a_1b_1 \cdots a_nb_n)$ in $(ab)^n \sqcup (ab)^n$, then every a_i and b_i can take 2 positions. This gives us the coefficient of $(a^2b^2)^n$ as $2^{2n} = 4^n$.

So, it is sufficient to show that there does not exist any other word except $(a^2b^2)^n$ on the left hand side. Since

$$\sum_{r=0}^{2n}(-1)^{n-r}|S_r| = \sum_{r=0}^{2n}(-1)^{n-r}\binom{4n}{2r} = 4^n$$

by Lemma 9 [Binomial coefficient 1], then we can conclude that the only remaining word on the left hand side is $(a^2b^2)^n$ and its coefficient is 4^n.

2.2.2 The coefficient of t^{4n+1}.

Let us find the coefficient of t^{4n+1} in the left hand side in Theorem 3 and show the equality between the coefficients on both side:

Lemma 2 . *The coefficient of t^{4n+1} in Theorem 3 is*

$$\frac{1}{4^n}\sum_{|r|\leq n}(-1)^r[(ab)^{n-r} \sqcup (ab)^{n+r}a] = (a^2b^2)^n a.$$

Proof. Let us investigate first several terms on the left hand side to find the pattern:

$$\begin{aligned}
& (\frac{t}{1+i})^5 ababa + (\frac{t}{1-i})(\frac{t}{1+i})^4(a \sqcup abab) + (\frac{t}{1-i})^2(\frac{t}{1+i})^3(ab \sqcup aba) \\
+ \quad & (\frac{t}{1-i})^3(\frac{t}{1+i})^2(aba \sqcup ab) + (\frac{t}{1-i})^4(\frac{t}{1+i})(abab \sqcup a) + (\frac{t}{1-i})^5 ababa \\
+ \quad & \cdots.
\end{aligned}$$

The shuffle operation is commutative and we have the following computations: $(\frac{1}{1-i})^5 = \frac{-1-i}{8}$, $(\frac{1}{1-i})^4(\frac{1}{1+i})^1 = \frac{-1+i}{8}$, $(\frac{1}{1-i})^3(\frac{1}{1+i})^2 = \frac{1+i}{8}$, $(\frac{1}{1-i})^2(\frac{1}{1+i})^3 = \frac{1-i}{8}$, $(\frac{1}{1-i})^1(\frac{1}{1+i})^4 = \frac{-1-i}{8}$, and $(\frac{1}{1+i})^5 = \frac{-1+i}{8}$. Therefore we obtain the coefficient of t^{4n+1} as

$$\frac{1}{4^n} \sum_{|r| \leq n} (-1)^r [(ab)^{n-r} \sqcup (ab)^{n+r} a].$$

Putting $k = n - r$, we can rewrite the statement of the lemma as the following:

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

We will prove this statement.

Let S_k be the multi-set of all words as the result of $(ab)^k \sqcup (ab)^{2n-k} a$, for $0 \leq k \leq 2n$. Then we get the following inclusion by Lemma 7 [Inclusion of multi-set 2]: $S_0 \subset S_1 \subset \cdots \subset S_n$ and $S_{2n} \subset \cdots \subset S_n$. And so, every word on the left hand side is contained in S_n.

On the other hand, we know that $(a^2b^2)^n a$ is not contained in S_k for $0 \leq k \leq 2n$ and $k \neq n$. Consider the formation of $(a^2b^2)^n a$ in detail. If we let $(ab)^n a$ be $(a_1 b_1 \cdots a_n b_n) a_{n+1}$ in $(ab)^n \sqcup (ab)^n a$, then a_i and b_i, for $1 \leq i \leq n$, can take 2 positions. This gives us that the coefficient of $(a^2b^2)^n a$ is $2^{2n} = 4^n$.

So, it is sufficient to show that there does not exist any other word except $(a^2b^2)^n a$. Since

$$\sum_{r=0}^{2n} (-1)^{n-r}|S_r| = \sum_{r=0}^{2n} (-1)^{n-r} \begin{pmatrix} 4n+1 \\ 2r+1 \end{pmatrix} = 4^n$$

by Lemma 10 [Binomial coefficient 2], then the only remaining word on the left hand side is $(a^2b^2)^n a$ and its coefficient is 4^n.

2.2.3 The coefficient of t^{4n+2}.

Let us find the coefficient of t^{4n+2} in the left hand side in Theorem 3 and show the equality between the coefficients on both side:

Lemma 3 . *The coefficient of* t^{4n+2} *in Theorem 3 is*

$$\frac{1}{2 \cdot 4^n} \sum_{|r| \le n} (-1)^r [(ab)^{n-r} a \sqcup (ab)^{n+r} a] = (a^2b^2)^n a^2.$$

Proof. Let us investigate first several terms on the left hand side to find the pattern:

$$\begin{aligned} & (\frac{t}{1+i})^6 ababab + (\frac{t}{1-i})(\frac{t}{1+i})^5 (a \sqcup ababa) + (\frac{t}{1-i})^2 (\frac{t}{1+i})^4 (ab \sqcup abab) \\ + & (\frac{t}{1-i})^3 (\frac{t}{1+i})^3 (aba \sqcup aba) + (\frac{t}{1-i})^4 (\frac{t}{1+i})^2 (abab \sqcup ab) \\ + & (\frac{t}{1-i})^5 (\frac{t}{1+i})(ababa \sqcup a) + (\frac{t}{1-i})^6 + \cdots. \end{aligned}$$

The shuffle operation is commutative and we have the following computations: $(\frac{1}{1-i})^6 = \frac{-i}{8}$, $(\frac{1}{1-i})^5(\frac{1}{1+i})^1 = \frac{-1}{8}$, $(\frac{1}{1-i})^4(\frac{1}{1+i})^2 = \frac{i}{8}$, $(\frac{1}{1-i})^3(\frac{1}{1+i})^3 = \frac{1}{8}$, $(\frac{1}{1-i})^2(\frac{1}{1+i})^4 = \frac{-i}{8}$, $(\frac{1}{1-i})^1(\frac{1}{1+i})^5 = \frac{-1}{8}$, and $(\frac{1}{1+i})^6 = \frac{i}{8}$. Therefore we obtain the coefficient of t^{4n+2} as

$$\frac{1}{2 \cdot 4^n} \sum_{|r| \le n} (-1)^r [(ab)^{n-r} a \sqcup (ab)^{n+r} a].$$

Putting $k = n-r$, we can rewrite the statement of the lemma as the following:

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

We will prove this statement.

Let S_k be the multi-set of all words as the result of $(ab)^k a \sqcup (ab)^{2n-k} a$, for $0 \leq k \leq n$. Then we get the following inclusion by Lemma 7 [Inclusion of multi-set 2]: $S_0 \subset S_1 \subset \cdots \subset S_n$. Since the shuffle operation is commutative, then $S_{2n-k} = S_k$. And so, every word on left hand side is contained in S_n.

On the other hand, we know that $(a^2b^2)^n a^2$ is not contained in S_k for $0 \leq k \leq 2n$ and $k \neq n$. Consider the formation of $(a^2b^2)^n a^2$ in detail. If we let $(ab)^n a$ be $(a_1 b_1 \cdots a_n b_n) a_{n+1}$ in $(ab)^n a \sqcup (ab)^n a$, then every a_i and b_i can take 2 positions. This gives us that the coefficient of $(a^2b^2)^n a^2$ is $2^{2n+1} = 2 \cdot 4^n$.

So, it is sufficient to show that there does not exist any other word except $(a^2b^2)^n a^2$ on the left hand side. Since

$$\sum_{r=0}^{2n} (-1)^{n-r} |S_r| = \sum_{r=0}^{2n} (-1)^{n-r} \begin{pmatrix} 4n+2 \\ 2r+1 \end{pmatrix} = 2 \cdot 4^n$$

by Lemma 11 [Binomial coefficient 3], then the only remaining word on left hand side is $(a^2b^2)^n a^2$ and its coefficient is $2 \cdot 4^n$.

2.2.4 The coefficient of t^{4n+3}.

Let us find the coefficient of t^{4n+3} in the left hand side in Theorem 3 and show the equality between the coefficients on both side:

Lemma 4 . *The coefficient of t^{4n+3} in Theorem 3 is*

$$\frac{1}{2\cdot 4^n}\sum_{r=-n}^{n+1}(-1)^r[(ab)^{n-r}ab \sqcup (ab)^{n+r}a] = (a^2b^2)^n a^2 b.$$

Proof. Let us investigate first several terms on the left hand side to find a pattern:

$$\begin{aligned} &(\frac{t}{1+i})^7 abababa + (\frac{t}{1-i})(\frac{t}{1+i})^6(a \sqcup ababab) + (\frac{t}{1-i})^2(\frac{t}{1+i})^5(ab \sqcup ababa) \\ + \ &(\frac{t}{1-i})^3(\frac{t}{1+i})^4(aba \sqcup abab) + (\frac{t}{1-i})^4(\frac{t}{1+i})^3(abab \sqcup aba) \\ + \ &(\frac{t}{1-i})^5(\frac{t}{1+i})^2(ababa \sqcup ab) + (\frac{t}{1-i})^6(\frac{t}{1+i})(ababab \sqcup a) \\ + \ &(\frac{t}{1-i})^7 abababa + \cdots. \end{aligned}$$

The shuffle operation is commutative and we have the following computations: $(\frac{1}{1-i})^7 = \frac{1-i}{16}$, $(\frac{1}{1-i})^6(\frac{1}{1+i})^1 = \frac{-1-i}{16}$, $(\frac{1}{1-i})^5(\frac{1}{1+i})^2 = \frac{-1+i}{16}$, $(\frac{1}{1-i})^4(\frac{1}{1+i})^3 = \frac{1+i}{16}$, $(\frac{1}{1-i})^3(\frac{1}{1+i})^4 = \frac{1-i}{16}$, $(\frac{1}{1-i})^2(\frac{1}{1+i})^5 = \frac{-1-i}{16}$, $(\frac{1}{1-i})^1(\frac{1}{1+i})^6 = \frac{-1+i}{16}$, $(\frac{1}{1+i})^7 = \frac{1+i}{16}$. Therefore we obtain the coefficient of t^{4n+3} on the left hand side as

$$\frac{1}{2\cdot 4^n}\sum_{r=-n}^{n+1}(-1)^r[(ab)^{n-r}ab \sqcup (ab)^{n+r}a].$$

Putting $k = n - r$, we can rewrite the statement of lemma as the following:

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

We will prove this statement:

Let S_k be the multi-set of all words as the result of $(ab)^{2n-k}ab \sqcup (ab)^k a$, for $0 \le k \le 2n$. Then we get the following inclusion by Lemma 7 [Inclusion of multi-set 2]: $S_0 \subset S_1 \subset \cdots \subset S_n$ and $S_{2n+1} \subset \cdots \subset S_n$. And so, every word on the left hand side is contained in S_n.

On the other hand, we know that $(a^2b^2)^n a^2 b$ is not contained in S_k for $0 \le k \le 2n+1$ and $k \ne n$. Consider the formation of $(a^2b^2)^n a^2 b$ in detail. If we let $(ab)^{n+1}$ be $(a_1b_1\cdots a_nb_n)a_{n+1}b_{n+1}$ in $(ab)^n a \sqcup (ab)^{n+1}$, then every a_i and b_i except b_{n+1} can take 2 positions. This gives us that the coefficient of $(a^2b^2)^n a^2 b$ is $2^{2n+1} = 2 \cdot 4^n$.

So, it is sufficient to show that there does not exist any other word except $(a^2b^2)^n a^2 b$ on the left hand side. Since

$$\sum_{r=0}^{2n+1} (-1)^{n-r} |S_k| = \sum_{r=0}^{2n+1} (-1)^{n-r} \binom{4n+3}{2r+1} = 2 \cdot 4^n$$

by Lemma 12 [Binomial coefficient 4], then the only remaining word on the left hand side is $(a^2b^2)^n a^2 b$ and its coefficient is $2 \cdot 4^n$.

2.2.5 Connection between Proposition 1 and Lemma 1.

Even though Proposition 1 and Theorem 3 are proved in different ways, that is, Proposition 1 is proved using an analytical method such as solving a differential equation with initial conditions, while Theorem 3 is proven, using combinatorial methods such as using the shuffle operation, there is a connection between Proposition 1 and Theorem 3:

In fact, Proposition 1 plays the same role as Lemma 1. Let us derive Proposition 1 from Lemma 1:

Lemma 1 says

$$\sum_{r=0}^{2n} (-1)^{n-r} [(ab)^r \sqcup (ab)^{2n-r}] = 4^n (a^2b^2)^n.$$

If we let a and b be any differential forms whose integrals converge, then

$$\sum_{r=0}^{2n} (-1)^r z^{4n} \int_0^x (ab)^r \int_0^x (ab)^{2n-r} = (-1)^n z^{4n} \int_0^x (4a^2b^2)^n,$$

obtained by multiplying with z^{4n} and taking integrals of both sides over the interval [0,x].

Taking a summation of both sides gives us the following:

$$\sum_{n\geq 0}(-1)^n z^{4n}\int_0^x (4a^2b^2)^n = \sum_{n\geq 0}\sum_{r=0}^{2n}(-1)^r z^{4n}\int_0^x (ab)^r\int_0^x (ab)^{2n-r}$$
$$= \sum_{k\geq 0}(-1)^k z^{2k}\int_0^x (ab)^k \sum_{m\geq 0} z^{2m}\int_0^x (ab)^m.$$

Hence Formula 2 can be also derived from Lemma 1.

2.3 Combinatorial identity 3 for multiple polylogarithms.

Theorem 4 .

$$\sum_{|r|\leq n}(-1)^r\{(ab)^{n-r}\sqcup(ba)^{n+r}\} = 2\cdot 4^{n-1}\{(abba)^n + (baab)^n\}.$$

Proof. Let $k = n-r$, then we can rewrite the left hand side as the following:

$$\sum_{k=0}^{2n}(-1)^{n-k}\{(ab)^k\sqcup(ba)^{2n-k}\}$$

We will show that this is equal to the right hand side. Let S_k be the multi-set of all words as the result of $(ab)^k\sqcup(ba)^{2n-k}$, for $0\leq k\leq n$. Then we get the following inclusion by Lemma 8 [Inclusion of multi-set 3]:$S_0\subset S_1\subset\cdots\subset S_n$. Since the shuffle operation is commutative, then $S_{2n-k} = S_k$. And so, every word on the left hand side is contained in S_n.

Let us look at the words on the right hand side. From the formation, we know that $(abba)^n$ and $(baab)^n$ are not contained in S_k for $0\leq k\leq 2n$ and $k\neq n$. Consider the formation of $(abba)^n$ in detail. Let $(ba)^n$ be $(b_1a_1b_2a_2\cdots b_na_n)$ in $(ab)^n\sqcup(ba)^n$. Then every a_j and b_j except a_n can take 2 positions and a_n must be fixed at the end. Similarly, when forming $(baab)^n$ in $(ab)^n \sqcup (b_1a_1b_2a_2\cdots b_na_n)$, every a_j and b_j except b_1 can take 2 positions and b_1 must be fixed in the first position. From these choices, we get that the coefficients of $(abba)^n$ and $(baab)^n$ are $2^{2n-1} = 2\cdot 4^{n-1}$.

So, it is sufficient to show that there does not exist any other word except $(abba)^n$ and $(baab)^n$. Since

$$\sum_{r=0}^{2n}(-1)^{n-r}|S_r| = \sum_{r=0}^{2n}(-1)^{n-r}\begin{pmatrix} 4n \\ 2r \end{pmatrix} = 4^n,$$

by Lemma 9 [Binomial coefficient 1], the only remaining terms on the left hand side are $(abba)^n$ and $(baab)^n$ and the coefficients are $2\cdot 4^{n-1}$.

2.3.1 Formula(1) from identity 3.

Even though Theorem 4 was proven using a combinatorial method, unfortunately, a and b cannot be any differential forms. For instance, if the iterated integral starts with $a = \frac{dx}{x}$ and $b = \frac{dx}{1-x}$, then the integral is divergent because the series starting with $b = \int_0^1 \frac{dx}{1-x}$ and ending with $a = \int_0^{x_n} \frac{dx}{x}$ are divergent.

But it does not mean that there do not exist any analytic formulas. Let us try to find analytic formulas putting a and b as differential forms whose integrals converge:

Let $a = \frac{\gamma dx}{1-\frac{x}{\alpha}}$ and $b = \frac{\delta dx}{1-\frac{x}{\beta}}$ where $\alpha,\beta,\gamma,\delta \in \mathbf{C}$, $|\alpha| > 1$, and $|\beta| > 1$, then we obtain the following formula:

Formula 5 .

$$\sum_{|r|\leq n}(-1)^r[\zeta(1,1,\{1,1\}^{n-r-1};\frac{1}{\alpha},\frac{\alpha}{\beta},\{\frac{\beta}{\alpha},\frac{\alpha}{\beta}\}^{n-r-1})$$
$$\cdot\zeta(1,1,\{1,1\}^{n+r-1};\frac{1}{\beta},\frac{\beta}{\alpha},\{\frac{\alpha}{\beta},\frac{\beta}{\alpha}\}^{n+r-1})]$$
$$= 2\cdot 4^{n-1}[\zeta(1,1,1,1,\{1,1,1,1\}^{n-1};\frac{1}{\alpha},\frac{\alpha}{\beta},1,\frac{\beta}{\alpha},\{1,\frac{\alpha}{\beta},1,\frac{\beta}{\alpha}\}^{n-1})$$
$$+ \zeta(1,1,1,1,\{1,1,1,1\}^{n-1};\frac{1}{\beta},\frac{\beta}{\alpha},1,\frac{\alpha}{\beta},\{1,\frac{\beta}{\alpha},1,\frac{\alpha}{\beta}\}^{n-1})]$$

where $|\alpha|>1$ *and* $|\beta|>1$.

Proof. Let $a=\frac{\gamma dx}{1-\frac{x}{\alpha}}$ and $b=\frac{\delta dx}{1-\frac{x}{\beta}}$ where $\alpha,\beta,\gamma,\delta\in\mathbf{C}$, $|\alpha|>1$, and $|\beta|>1$; let us find the following integrals: $\int_0^1(abba)^n$, $\int_0^1(baab)^n$, $\int_0^1(ab)^n$, and $\int_0^1(ba)^n$. If we apply these results to Theorem 4, then we can get a formula.

To start, let us take an integral of *abba* over the interval [0,1]. Then we obtain the following using geometric series:

$$\int_0^1 abba=\int_0^1\frac{\gamma dx_1}{1-\frac{x_1}{\alpha}}\int_0^{x_1}\frac{\delta dx_2}{1-\frac{x_2}{\beta}}\int_0^{x_2}\frac{\delta dx_3}{1-\frac{x_3}{\beta}}\int_0^{x_3}\frac{\gamma dx_4}{1-\frac{x_4}{\alpha}}$$
$$=(\alpha\beta\gamma\delta)^2\sum_{k_4\geq1}\sum_{k_3\geq1}\sum_{k_2\geq1}\sum_{k_1\geq1}\frac{\alpha^{-k_1-k_4}\beta^{-k_2-k_3}}{(k_1)(k_1+k_2)(k_1+k_2+k_3)(k_1+k_2+k_3+k_4)}$$

If we put $n_4=k_1$, $n_3=k_1+k_2$, $n_2=k_1+k_2+k_3$, and $n_1=k_1+k_2+k_3+k_4$, then

$$\int_0^1 abba = (\alpha\beta\gamma\delta)^2\sum_{n_1>n_2>n_3>n_4>0}\frac{\alpha^{-n_1+n_2-n_4}\beta^{-n_2+n_4}}{n_1n_2n_3n_4}$$
$$= (\alpha\beta\delta\gamma)^2\zeta(1,1,1,1;\frac{1}{\alpha},\frac{\alpha}{\beta},1,\frac{\beta}{\alpha}).$$

Next, let us take the integral of $(abba)^2$ over the interval [0,1], to find a pattern. We obtain the following using geometric series:

$$\int_0^1(abba)^2=(\alpha\beta\gamma\delta)^4\sum_{k_8,\cdots,k_1\geq1}\frac{\alpha^{-(k_1+k_4+k_5+k_8)}\beta^{-(k_2+k_3+k_6+k_7)}}{k_1(k_1+k_2)\cdots(k_1+k_2+k_3+\cdots+k_8)}$$

If we put $n_8 = k_1$, $n_7 = k_1 + k_2$, $n_6 = k_1 + k_2 + k_3$, $\cdots$, $n_1 = k_1 + k_2 + k_3 + \cdots + k_8$, then we get the following:

$$\begin{aligned}\int_0^1 (abba)^2 &= (\alpha\beta\gamma\delta)^4 \sum_{n_1>n_2>\cdots>n_8>0} \frac{\alpha^{-(n_1-n_2+n_4-n_6+n_8)}\beta^{-(n_2-n_4+n_6-n_8)}}{n_1 n_2 \cdots n_8} \\ &= (\alpha\beta\gamma\delta)^4 \zeta(1,1,1,1,1,1,1,1;\frac{1}{\alpha},\frac{\alpha}{\beta},1,\frac{\beta}{\alpha},1,\frac{\alpha}{\beta},1,\frac{\beta}{\alpha}).\end{aligned}$$

For the general case $\int_0^1 (abba)^n$ over the interval [0,1]. Then we get the following using geometric series :

$$\int_0^1 (abba)^n = (\alpha\beta\gamma\delta)^{2n} \sum_{k_{4n},\cdots,k_1 \geq 1} \frac{\alpha^{-(\sum_{m\geq 1}(k_{4m-3}+k_{4m}))}\beta^{-(\sum_{m\geq 1}(k_{4m-2}+k_{4m-1}))}}{\prod_{m\geq 1}\sum_{l=1}^{m} k_l}.$$

If we put $n_{4n} = k_1$, $n_{4n-1} = k_1 + k_2$, $\cdots$, $n_1 = \sum_{m=1}^{4n} k_m$ as we did for the case $(abba)^2$, then we can change the previous sums into the following sums. After that, we can convert the sums into multiple zeta values using the definition of multiple zeta values:

$$\begin{aligned}&\int_0^1 (abba)^n \\ &= (\alpha\beta\gamma\delta)^{2n} \sum_{n_1>n_2>\cdots>n_{4n}>0} \frac{\alpha^{-(n_1+\sum_{m=1}^{n}(-n_{4m-2}+n_{4m}))}\beta^{-(\sum_{m=1}^{n}(n_{4m-2}-n_{4m}))}}{\prod_{m=1}^{4n} n_m} \\ &= (\alpha\beta\gamma\delta)^{2n}\zeta(1,1,1,1,\{1,1,1,1\}^{n-1};\frac{1}{\alpha},\frac{\alpha}{\beta},1,\frac{\beta}{\alpha},\{1,\frac{\alpha}{\beta},1,\frac{\beta}{\alpha}\}^{n-1}).\end{aligned}$$

Symmetrically, we can get the following for the general case $(baab)^n$:

$$\int_0^1 (baab)^n = (\alpha\beta\gamma\delta)^{2n}\zeta(1,1,1,1,\{1,1,1,1\}^{n-1};\frac{1}{\beta},\frac{\beta}{\alpha},1,\frac{\alpha}{\beta},\{1,\frac{\beta}{\alpha},1,\frac{\alpha}{\beta}\}^{n-1}).$$

Let us investigate the left hand side in the same way. To begin, to find the pattern, let us look at some simple cases.

If we take an integral of (ab) over the interval [0,1], then we can get the following using geometric series:

$$\begin{aligned}\int_0^1 (ab) &= \int_0^1 \frac{\gamma dx_1}{1-\frac{x_1}{\alpha}} \int_0^{x_1} \frac{\delta dx_2}{1-\frac{x_2}{\beta}} \\ &= (\alpha\beta\gamma\delta) \sum_{k_2 \geq 1} \sum_{k_1 \geq 1} \frac{\alpha^{-k_2}\beta^{-k_1}}{k_1(k_1+k_2)}.\end{aligned}$$

If we put $n_2 = k_1$ and $n_1 = k_1 + k_2$, then we can obtain another sum different from the previous sums. By the definition of multiple zeta values, we get the following:

$$\begin{aligned}\int_0^1 (ab) &= (\alpha\beta\gamma\delta) \sum_{n_1 > n_2 > 0} \frac{\alpha^{-n_1+n_2}\beta^{-n_2}}{n_1 n_2} \\ &= (\alpha\beta\gamma\delta)\zeta(1,1;\frac{1}{\alpha},\frac{\alpha}{\beta}).\end{aligned}$$

Let us take the integral of $(ab)^2$ over the interval [0,1] to find the pattern, then we get the following using geometric series:

$$\begin{aligned}\int_0^1 (ab)^2 &= \int_0^1 \frac{\gamma dx_1}{1-\frac{x_1}{\alpha}} \int_0^{x_1} \frac{\delta dx_2}{1-\frac{x_2}{\beta}} \int_0^{x_2} \frac{\gamma dx_3}{1-\frac{x_3}{\alpha}} \int_0^{x_3} \frac{\delta dx_4}{1-\frac{x_4}{\beta}} \\ &= (\alpha\beta\gamma\delta)^2 \sum_{k_4,k_3,k_2,k_1 \geq 1} \frac{\alpha^{-(k_2+k_4)}\beta^{-(k_1+k_3)}}{k_1(k_1+k_2)(k_1+k_2+k_3)(k_1+k_2+k_3+k_4)}.\end{aligned}$$

If we put $n_4 = k_1$, $n_3 = k_1 + k_2$, $n_2 = k_1 + k_2 + k_3$, and $n_1 = k_1 + k_2 + k_3 + k_4$, then we can get the following in the same way as for the case (ab)

$$\begin{aligned}\int_0^1 (ab)^2 &= (\alpha\beta\gamma\delta)^2 \sum_{n_1 > n_2 > n_3 > n_4 > 0} \frac{\alpha^{-(n_1-n_2+n_3-n_4)}\beta^{-(n_2-n_3+n_4)}}{n_1 n_2 n_3 n_4} \\ &= (\alpha\beta\gamma\delta)^2\zeta(1,1,1,1;\frac{1}{\alpha},\frac{\alpha}{\beta},\frac{\beta}{\alpha},\frac{\alpha}{\beta}).\end{aligned}$$

Let us take an integral of the general case $(ab)^n$ over the interval [0,1]. Then we get the following using geometric series:

$$\int_0^1 (ab)^n = (\alpha\beta\gamma\delta)^n \sum_{k_{2n},\cdots,k_1 > 0} \frac{\alpha^{-(\sum_{m=1}^{n} k_{2m})}\beta^{-(\sum_{m=1}^{n} k_{2m-s})}}{\prod_{m=1}^{2n} \sum_{l=1}^{m} k_l}$$

If we put $n_{2n} = k_1$, $n_{2n-1} = k_1 + k_2$, $\cdots$, and $n_1 = \sum_{m=1}^{2n} k_m$, then we get the following by the definition of multiple zeta values:

$$\begin{aligned}\int_0^1 (ab)^n &= (\alpha\beta\gamma\delta)^n \sum_{n_1>n_2>\cdots>n_{2n}>0} \frac{\alpha^{-\sum_{m=1}^{2n}(-1)^{m+1}n_m}\beta^{-(\sum_{m=2}^{2n}(-1)^m n_m)}}{\prod_{m=1}^{2n} n_m} \\ &= (\alpha\beta\gamma\delta)^n \zeta(1,1,\{1,1\}^{n-1}; \frac{1}{\alpha}, \frac{\alpha}{\beta}, \{\frac{\beta}{\alpha}, \frac{\alpha}{\beta}\}^{n-1}).\end{aligned}$$

Symmetrically, we get the following for the case $(ba)^n$:

$$\int_0^1 (ba)^n = (\alpha\beta\gamma\delta)^n \zeta(1,1,\{1,1,\}^{n-1}; \frac{1}{\beta}, \frac{\beta}{\alpha}, \{\frac{\alpha}{\beta}, \frac{\beta}{\alpha}\}^{n-1}).$$

If we apply these results to Theorem 4 and cancel the $(\alpha\beta\gamma\delta)^{2n}$ on both sides, we get the following formula:

$$\begin{aligned}L.H.S &= \sum_{|r|\le n} (-1)^r \{\int_0^1 (ab)^{n-r} \int_0^1 (ba)^{n+r}\} \\ &= \sum_{|r|\le n} (-1)^r [\zeta(1,1,\{1,1\}^{n-r-1}; \frac{1}{\alpha}, \frac{\alpha}{\beta}, \{\frac{\beta}{\alpha}, \frac{\alpha}{\beta}\}^{n-r-1}) \\ &\quad \cdot \zeta(1,1,\{1,1\}^{n+r-1}; \frac{1}{\beta}, \frac{\beta}{\alpha}, \{\frac{\alpha}{\beta}, \frac{\beta}{\alpha}\}^{n+r-1})] \\ &= 2\cdot 4^{n-1}[\zeta(1,1,1,1,\{1,1,1,1\}^{n-1}; \frac{1}{\alpha}, \frac{\alpha}{\beta}, 1, \frac{\beta}{\alpha}, \{1, \frac{\alpha}{\beta}, 1, \frac{\beta}{\alpha}\}^{n-1}) \\ &+ \zeta(1,1,1,1,\{1,1,1,1\}^{n-1}; \frac{1}{\beta}, \frac{\beta}{\alpha}, 1, \frac{\alpha}{\beta}, \{1, \frac{\beta}{\alpha}, 1, \frac{\alpha}{\beta}\}^{n-1})] \\ &= 2\cdot 4^{n-1}\{\int_0^1 (abba)^n + \int_0^1 (baab)^n\} = R.H.S.\end{aligned}$$

2.3.2 Formula(2) from identity 3.

If we put $a = x^{\alpha-1}dx$ and $b = x^{\beta-1}dx$ where $\alpha\cdot\beta \neq 0$, $\alpha+\beta \neq 0$, $m\alpha + (m+1)\beta \neq 0$, $(m+1)\alpha + m\beta \neq 0$, and $m \in \mathbf{Z}$, then we obtain another formula. Moreover, this formula is related to rational functions, which means that our identities can derive other formulas, that are not related to multiple zeta functions:

Formula 6 .

$$\sum_{|r|\le n}(-1)^r[\prod_{j=1}^{n-r}\frac{1}{j\{(j-1)\alpha+j\beta\}}\cdot\prod_{j=1}^{n+r}\frac{1}{j\{j\alpha+(j-1)\beta\}}]$$

$$= 2\cdot 4^{n-1}\prod_{j=1}^{n-r}\frac{1}{j(j+1)}[\frac{1}{\{j\alpha+(j-1)\beta\}\cdot\{j\alpha+(j+1)\beta\}}$$

$$+ \frac{1}{\{(j-1)\alpha+j\beta\}\cdot\{(j+1)\alpha+j\beta\}}]$$

where $\alpha\cdot\beta\neq 0$, $\alpha+\beta\neq 0$, $m\alpha+(m+1)\beta\neq 0$, $(m+1)\alpha+m\beta\neq 0$, *and* $m\in\mathbf{Z}$.

Proof. Let $a = x^{\alpha-1}dx$ and $b = x^{\beta-1}dx$ where $\alpha\cdot\beta\neq 0$, $\alpha+\beta\neq 0$, $m\alpha+(m+1)\beta\neq 0$, $(m+1)\alpha+m\beta\neq 0$, and $m\in\mathbf{Z}$; let us find the following integrals: $\int_0^1(abba)^n$, $\int_0^1(baab)^n$, $\int_0^1(ab)^n$, and $\int_0^1(ba)^n$. If we apply these results to Theorem 4, then we get a formula.

To start, let us take the integral of $(ab)^n$ over the interval [0,1]. Then we get the following:

$$\begin{aligned}\int_0^1(ab)^n &= \int_0^1 x_1^{\alpha-1}dx_1\int_0^{x_1}x_2^{\beta-1}dx_2\\ &\cdots\int_0^{x_{2n-2}}x_{2n-1}^{\alpha-1}dx_{2n-1}\int_0^{x_{2n-1}}x_{2n}^{\beta-1}dx_{2n}\\ &= \int_0^1 x_1^{\alpha-1}dx_1\int_0^{x_1}x_2^{\beta-1}dx_2\\ &\cdots\int_0^{x_{2n-2}}x_{2n-1}^{\alpha-1}\frac{x_{2n-1}^{\beta}}{\beta}dx_{2n-1}\\ &= \prod_{j=1}^{n}\frac{1}{\{(j-1)\alpha+j\beta\}\{j\alpha+j\beta\}}\\ &= \frac{1}{(\alpha+\beta)^n}\prod_{j=1}^{n}\frac{1}{j\{j\alpha+(j-1)\beta\}}.\end{aligned}$$

Symmetrically, we can get the following result for the case $(ba)^n$:

$$\int_0^1(ba)^n = \frac{1}{(\alpha+\beta)^n}\prod_{j=1}^{n}\frac{1}{j\{j\alpha+(j-1)\beta\}}.$$

Let us look at the right hand side: If we take the integral of $(abba)$ over the interval [0,1], then we can easily obtain a pattern.

$$\begin{aligned}\int_0^1 abba &= \int_0^1 x_1^{\alpha-1}dx_1 \int_0^{x_1} x_2^{\beta-1}\frac{x_2^{\alpha+\beta}}{\alpha(\alpha+\beta)}dx_2 \\ &= \frac{x_1^{2\alpha+2\beta}}{\alpha(\alpha+\beta)(\alpha+2\beta)(2\alpha+2\beta)}\Big|_0^1 \\ &= \frac{1}{\alpha(\alpha+\beta)(\alpha+2\beta)(2\alpha+2\beta)} \\ &= \frac{1}{1\cdot 2(\alpha+\beta)^2\alpha(\alpha+2\beta)}.\end{aligned}$$

If we take the integral of $(abba)^n$ over the interval [0,1], then we obtain the following result:

$$\int_0^1 (abba)^n = \frac{1}{(\alpha+\beta)^{2n}}\prod_{j=1}^{n}\frac{1}{j(j+1)\{j\alpha+(j-1)\beta\}\{j\alpha+(j+1)\beta\}}.$$

Symmetrically, we get the following result taking the integral of $(baab)^n$ over the interval [0,1]:

$$\int_0^1 (baab)^n = \frac{1}{(\alpha+\beta)^{2n}}\prod_{j=1}^{n}\frac{1}{j(j+1)\{(j-1)\alpha+j\beta\}\{(j+1)\alpha+j\beta\}}.$$

If we apply these results to The Theorem 4 and cancel $\frac{1}{(\alpha+\beta)^{2n}}$, then we get the following:

$$\begin{aligned}L.H.S &= \sum_{|r|\le n}(-1)^r\{\int_0^1 (ab)^{n-r}\int_0^1 (ba)^{n+r}\} \\ &= \sum_{|r|\le n}(-1)^r[\prod_{j=1}^{n-r}\frac{1}{j\{(j-1)\alpha+j\beta\}}\cdot\prod_{j=1}^{n+r}\frac{1}{j\{j\alpha+(j-1)\beta\}}] \\ &= 2\cdot 4^{n-1}\prod_{j=1}^{n-r}\frac{1}{j(j+1)}[\frac{1}{\{j\alpha+(j-1)\beta\}\cdot\{j\alpha+(j+1)\beta\}} \\ &+ \frac{1}{\{(j-1)\alpha+j\beta\}\cdot\{(j+1)\alpha+j\beta\}}] \\ &= 2\cdot 4^{n-1}\{\int_0^1 (abba)^n + \int_0^1 (baab)^n\} = R.H.S.\end{aligned}$$

Remark. If we put $a = e^{-\alpha t}dt$ and $b = e^{-\beta t}dt$, where $|\alpha| > 0$ and $|\beta| > 0$, and take the integrals of both sides over the interval $[0, \infty]$, then we also can get the same result as Formula 6. If we put $x = e^t$ in the setting of Formula 6, we can derive Formula 6 from this setting.

2.4 Combinatorial identity 4 for multiple polylogarithms.

Let a base be $\underbrace{\overbrace{aaaabb}^{1\ unit}aaaabb\cdots aaaabb}_{n\ units} = (a^4b^2)^n$. Then the base is in the multi-set S_n coming from $(a^2b)^n \sqcup (a^2b)^n$.

We define $\left\{\begin{matrix} 2n-1 \\ 2n-j \end{matrix}\right\}$ by $(2n-j)$ transpositions between $'b'$s with their closest $'a'$ on the base

$$(a^4b^2)^n = \underbrace{\overbrace{aaaabb}^{1\ unit}aaaabb\cdots aaaabb}_{n\ units}.$$

Then the number of words in $\left\{\begin{matrix} 2n-1 \\ 2n-j \end{matrix}\right\}$ is $\begin{pmatrix} 2n-1 \\ 2n-j \end{pmatrix}$.

Let us look at examples of $\left\{\begin{matrix} 2n-1 \\ 2n-j \end{matrix}\right\}$.

Example 2.4.1. In case $n = 3$, $\left\{\begin{matrix} 5 \\ 1 \end{matrix}\right\}$ denotes one transposition between $'b'$ and its closest $'a'$ on the base $(a^4b^2)^3 = aaaabbaaaabbaaaabb$, that is,

$$\begin{aligned} \left\{\begin{matrix} 5 \\ 1 \end{matrix}\right\} &= (a^3baba^4b^2a^4b^2 + a^4baba^3b^2a^4b^2 + a^4b^2a^3baba^4b^2 \\ &+ a^4b^2a^4baba^3b^2 + a^4b^2a^4b^2a^3bab). \end{aligned}$$

*Example*2.4.2. In the case $n = 3$, $\left\{\begin{matrix} 5 \\ 2 \end{matrix}\right\}$ denotes two transpositions between

$'b'$s and their closest $'a'$ on the base $(a^4b^2)^3$, respectively. Then the number of terms is $\begin{pmatrix} 5 \\ 2 \end{pmatrix}$=10.

Theorem 7 .

$$\sum_{|r|\leq n} (-1)^r[(a^2b)^{n-r} \sqcup (a^2b)^{n+r}] = 3^n \sum_{j=1}^{2n} 2^j \begin{Bmatrix} 2n-1 \\ 2n-j \end{Bmatrix}.$$

Proof. To begin with, we can rewrite the left hand side as follows, by putting $k = n - r$:

$$\sum_{k=0}^{2n}(-1)^{n-k}\{(a^2b)^k \sqcup (a^2b)^{2n-k}\}$$

We will show that it is equal to the right hand side.

Let S_k be the multi-set of all words coming from $(a^2b)^k \sqcup (a^2b)^{2n-k}$, for $0 \leq k \leq n$. Then we can get the following inclusion by Lemma 6 [Inclusion of multi-set 1]: $S_0 \subset S_1 \subset \cdots \subset S_n$. Since the shuffle operation is commutative, then $S_{2n-k} = S_k$. Hence every word on the left hand side is contained in S_n.

On the other hand, since the number of elements of S_k is $\begin{pmatrix} 6n \\ 3k \end{pmatrix}$, then, by Lemma 13 [Binomial coefficient 5], we get the following:

$$\begin{aligned} \sum_{k=0}^{2n}(-1)^{n-k}|S_k| &= \sum_{k=0}^{2n}(-1)^{n-k} \begin{pmatrix} 6n \\ 3k \end{pmatrix} \\ &= 3^n \sum_{j=0}^{2n} 2^j \begin{pmatrix} 2n-1 \\ 2n-j \end{pmatrix}, \end{aligned}$$

where $|S_k|$ is the number of elements of S_k.

Therefore, to complete the proof of Theorem 7, we have to show that every word on the right hand side is contained in S_n and the coefficient of every word in $\left\{ \begin{array}{c} 2n-1 \\ 2n-j \end{array} \right\}$ is $3^n \cdot 2^j$. The first statement is obvious from the formations of the words.

To show the second statement, we will use the following strategy: First, we investigate several beginning terms. This investigation reveals a pattern of the coefficients of terms on the right hand side. Secondly, from the pattern, we will formulate a lemma of the formation that states the general rule. Finally, we will prove the lemma.

Let us investigate first several terms to find a pattern of the coefficients of terms on the right hand side:

For

$$3^n 2^{2n} \left\{ \begin{array}{c} 2n-1 \\ 0 \end{array} \right\} = 3^n 2^{2n} (a^4 b^2)^n,$$

each aab and AAB must be used to make a^4b^2 of the $(a^4b^2)^n$ in S_n if we put one $(aab)^n$ as $(AAB)^n$. And so, two $'A$'s can choose 3 positions with repeats and one $'B'$ can choose 2 positions in each unit a^4b^2. Hence, the coefficient (actually the number of choices) is $\begin{pmatrix} 4 \\ 2 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix} = 3 \cdot 2^2$.

This process must be repeated n-times to make $(a^4b^2)^n$. Therefore, the coefficient is $3^n 2^{2n}$, since $(a^4b^2)^n$ is contained in S_n, but not S_k for $0 \leq k < n$.

For

$$3^n 2^{2n-1} \left\{ \begin{matrix} 2n-1 \\ 1 \end{matrix} \right\},$$

since we have one transposition between $'b'$ and its closest $'a'$, the forms are of the following two types wherever the location of $'b'$ is:

$$\cdots a^3 baba^4 b^2 \cdots \tag{1}$$

$$\cdots a^4 baba^3 b^2 \cdots . \tag{2}$$

It does not matter where the location of $'b'$ is because the type is unique if we consider the broken a^4b^2 or $(a^4b^2)^2$, partially. Since the coefficient of words in $\left\{ \begin{matrix} 2n-1 \\ 1 \end{matrix} \right\}$ is $3^n 2^{2n-1}$, we need that the coefficient of (1) and (2) is $3^2 2^3$, because $3^{n-2} 2^{2(n-2)}$ comes from $(a^4b^2)^{n-2}$.

For

$$3^n 2^{2n-2} \left\{ \begin{matrix} 2n-1 \\ 2 \end{matrix} \right\},$$

since we have two transpositions between $'b'$ and its closest $'a'$, the forms are of the following types:

$$\cdots a^3 ba^2 ba^3 b^2 \cdots \tag{3}$$

$$\cdots a^4 baba^2 bab \cdots . \tag{4}$$

or the combination of two separated (1)s,(2)s, or (1) and (2) on a^4b^2s.

Wherever the locations of $'b'$s are, the types are unique if we consider the broken a^4b^2s partially. Since the coefficient of terms in $\left\{ \begin{matrix} 2n-1 \\ 2 \end{matrix} \right\}$ is $3^n 2^{2n-2}$, we need that the coefficient of (3) and (4) is $3^2 2^2$, because $3^{n-2}2^{2(n-2)}$ comes from $(a^4b^2)^{n-2}$.

For

$$3^n 2^{2n-3} \begin{Bmatrix} 2n-1 \\ 3 \end{Bmatrix},$$

since we have three transpositions between $'b'$ and its closest $'a'$, then the forms are of the following types:

$$\cdots a^3ba^2ba^2baba^4b^2\cdots, \qquad (5)$$

$$\cdots a^4baba^2ba^2ba^3b^2\cdots \qquad (6)$$

or the combination of (1) through (4).

Wherever the locations of the $'b'$s are, the types are unique if we consider the broken a^4b^2s partially. Since the coefficient of terms in $\begin{Bmatrix} 2n-1 \\ 3 \end{Bmatrix}$ is $3^n 2^{2n-3}$, we need that the coefficient of (5) and (6) is $3^3 2^3$, because $3^{n-3}2^{2(n-3)}$ comes from $(a^4b^2)^{n-3}$.

To make sure a pattern, let us look at the next case: For

$$3^n 2^{2n-3} \begin{Bmatrix} 2n-1 \\ 4 \end{Bmatrix},$$

since we have four transpositions between $'b'$ and its closest $'a'$, then the forms are of the following types:

$$\cdots a^3ba^2ba^2ba^2ba^3b^2\cdots, \qquad (7)$$

$$\cdots a^4baba^2ba^2ba^2bab\cdots, \qquad (8)$$

or the combination of (1) through (6).

In this case, since the coefficients of terms in $\left\{ \begin{matrix} 2n-1 \\ 4 \end{matrix} \right\}$ are $3^n 2^{2n-4}$, we need that the coefficient of (7) and (8) is $3^3 2^2$, because $3^{n-3}2^{2(n-3)}$ comes from $(a^4b^2)^{n-3}$. Wherever the locations of the $'b'$s are, the types are unique if we consider the broken a^4b^2s, partially.

From these examples, we can get a pattern described in the following lemma and complete the proof by proving the lemma.

2.4.1 Lemma for the coefficients.

Lemma 5 .

1. *If* $m = 2k+1$, $0 \le k \le n-1$, *then the coefficients of* $a^3b(a^2b)^{2k}aba^4b^2$ *and* $a^4bab(a^2b)^{2k}a^3b^2$ *are* $3^{k+2}2^3$.
2. *If* $m = 2s$, $1 \le s \le n$, *then the coefficients of* $a^3b(a^2b)^{2s-1}a^3b^2$ *and* $a^4bab(a^2b)^{2s-1}ab$ *are* $3^{s+1}2^2$

Proof. **Case 1-1:The coefficient of $a^3b(a^2b)^{2k}aba^4b^2$ is $3^{k+2}2^3$.**

Since $3 \cdot 2^2$ comes from a^4b^2, it's sufficient to show that the coefficient of $a^3b(a^2b)^{2k}ab$ is $3^{k+1}2$.

Here is the strategy for proving Case 1-1: First, it will be shown that it's true for several initial subcases. Secondly, we will find the pattern of coefficients and explain our notation from this investigation. Finally, the pattern will be proved.

If $k = 0$, then a^3bab comes from either $(aa \sqcup A)bAB$ or $(AA \sqcup a)Bab$ and the coefficient is $3 \cdot 2$. We will call this type of pair the symmetric case.

If $k = 1$, $a^3b(a^2b)^2ab$ comes from the following:

For $(aab)^2 \sqcup (AAB)^2$, the coefficient of $a^3b(a^2b)^2ab$ is $3^2 2^2$ from the following table:

Part A	Part B	Part C	CFC
$(aa \sqcup A)b$	$(a \sqcup A)B$	$\left\{ \begin{array}{c} (a \sqcup A)bAB \\ or\ AABab \end{array} \right\}$	by a symmetric case
↓	↓	↓	×2
3	2	3	$3^2 2^2$

Table 2.1. $a^3b(a^2b)^2ab$ (1)

There exists a symmetric case using $(AA \sqcup a)$ instead of $(aa \sqcup A)$ in Part A. So, the sub-total coefficient is $3^2 2^2$ (CFC is denoted the Coefficient For each Cases).

For $(aab)^3 \sqcup (AAB)$ and $(aab) \sqcup (AAB)^3$ (we will also call this a symmetric case.), the coefficient of $a^3b(a^2b)^2ab$ is $3^2 2$ from the following table:

Part A	Part B	Part C	CFC
$(aa \sqcup A)b$	aab	$\left\{ \begin{array}{c} (a \sqcup A)Bab \\ or\ aabAB \end{array} \right\}$	by a symmetric case
↓	↓	↓	×2
3	1	3	$3^2 2$

Table 2.2. $a^3b(a^2b)^2ab$ (2)

There exists a symmetric case at $(aab) \sqcup (AAB)^3$. So, the sub-total coefficient is $3^2 2$. Therefore, the total coefficient of $a^3b(a^2b)^2ab$ is $3^2 2^2 - 3^2 2 = 3^2 2$.

To make sure the pattern is correct, let us investigate the subcase $k = 2$. Then the coefficient of $a^3b(a^2b)^4ab$ comes from the following table:

Part A	Part B	Part C	CFC
$(aa \sqcup A)b$	$(a \sqcup A)B(a \sqcup A)b(a \sqcup A)B$	$\left\{ (a \sqcup A)bAB \text{ or } AABab \right\}$	$3^2 2^3$
$(aa \sqcup A)b$	$aab(a \sqcup A)B(a \sqcup A)b$	$\left\{ (a \sqcup A)Bab \text{ or } aabAB \right\}$	$-3^2 2^2$
$(aa \sqcup A)b$	$(a \sqcup A)BAAB(a \sqcup A)b$	$\left\{ (a \sqcup A)Bab \text{ or } aabAB \right\}$	$+3^2 2^2$
$(aa \sqcup A)b$	$(a \sqcup A)B(a \sqcup A)baab$	$\left\{ (a \sqcup A)Bab \text{ or } aabAB \right\}$	$-3^2 2^2$
$(aa \sqcup A)b$	$aabaab(a \sqcup A)B$	$\left\{ (a \sqcup A)bAB \text{ or } AABab \right\}$	$-3^2 2$
$(aa \sqcup A)b$	$aab(a \sqcup A)BAAB$	$\left\{ (a \sqcup A)bAB \text{ or } AABab \right\}$	$+3^2 2$
$(aa \sqcup A)b$	$(a \sqcup A)BAABAAB$	$\left\{ (a \sqcup A)bAB \text{ or } AABab \right\}$	$-3^2 2$
$(aa \sqcup A)b$	$aabaabaab$	$\left\{ (a \sqcup A)Bab \text{ or } aabAB \right\}$	3^2

Table 2.3. $a^3b(a^2b)^4ab$

By symmetries, the total coefficient is $3^3 2$.

Let CUl be the case that the number of unbroken $aab(or AAB)$ in Part B is $2 \cdot l$; let CLl be the case that the number of unbroken $aab(or AAB)$ in Part B is $2 \cdot l + 1$. Then, in the formations of each case, the Number of Remaining Terms (denoted as NRT) and the coefficient for each case are in the following table.

All cases	NRT	CFC
CU0	$\binom{k-1}{0}$	$+3^2 2^{2k-1} \binom{k-1}{0}$
CL0	$\binom{k-1}{0}$	$-3^2 2^{2k-2} \binom{k-1}{0}$
CU1	$\binom{k-1}{1}$	$-3^2 2^{2k-3} \binom{k-1}{1}$
CL1	$\binom{k-1}{1}$	$+3^2 2^{2k-4} \binom{k-1}{1}$
⋮	⋮	⋮
CU(k-2)	$\binom{k-1}{k-2}$	$3^2 2^3 (-1)^{k-2} \binom{k-1}{k-2}$
CL(k-2)	$\binom{k-1}{k-2}$	$3^2 2^2 (-1)^{k-1} \binom{k-1}{k-2}$
CU(k-1)	$\binom{k-1}{k-1}$	$3^2 2^1 (-1)^{k-1} \binom{k-1}{k-1}$
CL(k-1)	$\binom{k-1}{k-1}$	$3^2 (-1)^k \binom{k-1}{k-1}$

Table 2.4. NRT and CFC of Case 1-1

Let us prove the following statement to prove the pattern: The NRT in the table CUl for k is $\begin{pmatrix} k-1 \\ l \end{pmatrix}$, and the NRT in the table CLl for k is $\begin{pmatrix} k-1 \\ l \end{pmatrix}$.

Let us think about the Part B; let us denote one of aab, AAB, $(a \sqcup A)b$, and $(a \sqcup A)B$ as a unit. CUl for k starts with the following form in Part B:

$$\underbrace{\overbrace{aabaab\cdots aab}^{2l\ units}(a \sqcup A)B(a \sqcup A)b\cdots(a \sqcup A)B}_{2k-1\ units}.$$

In the $2l$ units of aab, $(aab)^m$, for m even, can shift with an even number of $(a \sqcup A)b(or\ \ B)$, which means that if m is odd or m is even and odd shifting, then the terms are cancelled. For example,

$$w_1 = \underbrace{\overbrace{aab\cdots aab}^{2l-1\ units}(a \sqcup A)BAAB(a \sqcup A)b\cdots(a \sqcup A)B}_{2k-1\ units}.$$

is cancelled with $w_2 =$

$$\underbrace{\overbrace{aab\cdots aab}^{2l-1\ units}(a \sqcup A)B(a \sqcup A)baab(a \sqcup A)B\cdots(a \sqcup A)B}_{2k-1\ units},$$

for w_1 is in S_{k+l-2} and w_2 is in S_{k+l-1}.

$$w_3 = \underbrace{\overbrace{aab\cdots aab}^{2l-1\ units}(a \sqcup A)B(a \sqcup A)b\cdots(a \sqcup A)BAAB}_{2k-1\ units}.$$

is cancelled with $w_4 =$

$$\underbrace{\overbrace{aab\cdots aab}^{2l-1\ units}(a \sqcup A)BAABAAB(a \sqcup A)b\cdots(a \sqcup A)B}_{2k-1\ units},$$

for w_3 is in S_{k+l-2} and w_4 is in S_{k+l-3}.

Therefore to remain in the formation of a word, $(aab)^m$ can take the $k-l$ locations with repeats. Hence the number of remaining terms is $\begin{pmatrix} k-1 \\ l \end{pmatrix}$.

On the other hand, CLl for k starts with the following form in Part B:

$$\underbrace{\overbrace{aabaab\cdots aab}^{2l+1\ units}(a\sqcup A)B(a\sqcup A)b\cdots(a\sqcup A)b}_{2k-1\ units}.$$

In the $2l+1$ units of aab, $(aab)^m$, for m even, can shift with even number of $(a\sqcup A)b(or\ \ B)$, which means that if m is odd or m is even and odd shifting, then the terms are cancelled.

For example,

$$w_1 = \underbrace{\overbrace{aab\cdots aab}^{2l\ units}(a\sqcup A)BAAB(a\sqcup A)b\cdots(a\sqcup A)b}_{2k-1\ units}.$$

is cancelled with $w_2 =$

$$\underbrace{\overbrace{aab\cdots aab}^{2l\ units}(a\sqcup A)B(a\sqcup A)baab(a\sqcup A)B\cdots(a\sqcup A)b}_{2k-1\ units},$$

for w_1 is in S_{k+l-2} and w_2 is in S_{k+l-1} w_3

$$\underbrace{\overbrace{aab\cdots aab}^{2l-1\ units}(a\sqcup A)B(a\sqcup A)b\cdots AABAAB(a\sqcup A)b}_{2k-1\ units}.$$

is cancelled with $w_4 =$

$$\underbrace{\overbrace{aab\cdots aab}^{2l-1\ units}(a\sqcup A)B(a\sqcup A)b\cdots AAB(a\sqcup A)baab}_{2k-1\ units},$$

for w_3 is in S_{k+l-3} and w_2 is in S_{k+l-2}

Hence $(aab)^m$, for m even, can shift with even number of $(a \sqcup A)b(or\ B)$ and can take the $k-l$ locations with repeats. Hence the number of remaining terms is $\begin{pmatrix} k-1 \\ l \end{pmatrix}$.

Since the sum of CFC from the table is $2 \cdot 3^{k+1}$, from the following computation,

$$\begin{aligned}
& 2 \cdot 3^2[2^{2k-1}\begin{pmatrix} k-1 \\ 0 \end{pmatrix} - 2^{2k-2}\begin{pmatrix} k-1 \\ 0 \end{pmatrix} - 2^{2k-3}\begin{pmatrix} k-1 \\ 1 \end{pmatrix} \\
+ \ & 2^{2k-4}\begin{pmatrix} k-1 \\ 1 \end{pmatrix} + - - + \cdots + (-1)^{k-1}2^1\begin{pmatrix} k-1 \\ k-1 \end{pmatrix} + (-1)^k 2^0 \begin{pmatrix} k-1 \\ k-1 \end{pmatrix}] \\
= \ & 2 \cdot 3^2[2^{2k-2}\begin{pmatrix} k-1 \\ 0 \end{pmatrix} - 2^{2k-4}\begin{pmatrix} k-1 \\ 1 \end{pmatrix} + - \cdots + (-1)^k 2^0 \begin{pmatrix} k-1 \\ k-1 \end{pmatrix}] \\
= \ & 2 \cdot 3^2[4^{k-1}\begin{pmatrix} k-1 \\ k-1 \end{pmatrix} - 4^{k-2}\begin{pmatrix} k-1 \\ k-2 \end{pmatrix} + - \cdots + (-1)^{k-1} 4^0 \begin{pmatrix} k-1 \\ 0 \end{pmatrix}] \\
= \ & 2 \cdot 3^2 \sum_{l=0}^{k-1} \begin{pmatrix} k-1 \\ k-1-l \end{pmatrix} 4^{k-1-l}(-1)^l \\
= \ & 2 \cdot 3^2 3^{k-1} = 2 \cdot 3^{k+1},
\end{aligned}$$

we can complete the proof of Case 1-1: The coefficient of $a^3b(a^2b)^{2k}aba^4b^2$ is $3^{k+2}2^3$.

Case 1-2: The coefficient of $a^4bab(a^2b)^{2k}a^3b^2$ is $3^{k+2}2^3$.

Our strategy is equal to that of the proof of Case 1-1. Let us investigate subcases for Case 1-2.

If $k = 0$, then the coefficient of $a^4baba^3b^2$ comes from the following:

Part A	Part B	CFC
$(aa \sqcup AA)baB$	$(a \sqcup AA)(b \sqcup B)$	by a symmetric case
$\downarrow$	$\downarrow$	$\times 2$
6	6	$3^2 2^3$

Table 2.5. $a^4baba^3b^2$

If $k = 1$, then the coefficient of $a^4bab(a^2b)^2a^3b^2$ comes from the following:

Part A	Part B	Part C	CFC
$(aa \sqcup AA)baB$	$(a \sqcup A)b$	$\left\{ (a \sqcup A)B(a \sqcup AA)(b \sqcup B)\ \text{or}\ aab(A \sqcup aa)(b \sqcup B) \right\}$	$3^2 2^3$
$(aa \sqcup AA)baB$	AAB	$\left\{ (a \sqcup A)b(aa \sqcup A)(b \sqcup B)\ \text{or}\ AAB(AA \sqcup a)(b \sqcup B) \right\}$	$3^2 2^2$

Table 2.6. $a^4bab(a^2b)^2a^3b^2$

Therefore the sub-total of the coefficient is $3^3 2^2$. By symmetry, the coefficient of $a^4bab(a^2b)^2a^3b^2$ is $3^3 2^3$.

If $k = 2$, then the coefficient of $a^4bab(a^2b)^4a^3b^2$ comes from the following:

Part A	Part B	Part C	CFC
$(aa \sqcup AA)BAb$	$(a \sqcup A)B(a \sqcup A)b(a \sqcup A)B$	$\left\{ \begin{array}{c} (a \sqcup A)b(aa \sqcup A)(b \sqcup B) \\ or\ AAB(AA \sqcup a)(b \sqcup B) \end{array} \right\}$	$3^2 2^5$
$(aa \sqcup AA)BAb$	$aab(a \sqcup A)B(a \sqcup A)b$	$\left\{ \begin{array}{c} (a \sqcup A)B(AA \sqcup a)(B \sqcup b) \\ or\ aab(aa \sqcup A)(B \sqcup b) \end{array} \right\}$	$+3^2 2^4$
$(aa \sqcup AA)BAb$	$(a \sqcup A)BAAB(a \sqcup A)b$	$\left\{ \begin{array}{c} (a \sqcup A)B(AA \sqcup a)(B \sqcup b) \\ or\ aab(aa \sqcup A)(B \sqcup b) \end{array} \right\}$	$-3^2 2^4$
$(aa \sqcup AA)BAb$	$(a \sqcup A)B(a \sqcup A)baab$	$\left\{ \begin{array}{c} (a \sqcup A)B(AA \sqcup a)(B \sqcup b) \\ or\ aab(aa \sqcup A)(B \sqcup b) \end{array} \right\}$	$+3^2 2^4$
$(aa \sqcup AA)BAb$	$aabaab(a \sqcup A)B$	$\left\{ \begin{array}{c} (a \sqcup A)b(aa \sqcup A)(B \sqcup b) \\ or\ AAB(AA \sqcup a)(B \sqcup b) \end{array} \right\}$	$-3^2 2^3$
$(aa \sqcup AA)BAb$	$aab(a \sqcup A)BAAB$	$\left\{ \begin{array}{c} (a \sqcup A)b(aa \sqcup A)(B \sqcup b) \\ or\ AAB(AA \sqcup a)(B \sqcup b) \end{array} \right\}$	$+3^2 2^3$
$(aa \sqcup AA)BAb$	$(a \sqcup A)BAABAAB$	$\left\{ \begin{array}{c} (a \sqcup A)b(aa \sqcup A)(B \sqcup b) \\ or\ AAB(AA \sqcup a)(B \sqcup b) \end{array} \right\}$	$-3^2 2^3$
$(aa \sqcup AA)BAb$	$aabaabaab$	$\left\{ \begin{array}{c} (a \sqcup A)B(AA \sqcup a)(B \sqcup b) \\ or\ aab(aa \sqcup A)(B \sqcup b) \end{array} \right\}$	$-3^2 2^2$

Table 2.7. $a^4bab(a^2b)^4a^3b^2$

Therefore the sub-total of the coefficient is $3^4 2^2$. By symmetry, the coefficient is $3^4 2^3$.

Let us compare Case 1-1 and Case 1-2: The differences between Case 1-1 and Case 1-1 occur in Part A and Part C, which changes CFC. Here are the changes:

	Case 1-1	Change	Case 1-2
Part A	$(aa \sqcup A)b$	$\longrightarrow$	$(aa \sqcup AA)BAb$
CFC	3	$\longrightarrow$	$3 \cdot 2$
Part C	$\left\{ \begin{matrix} (a \sqcup A)bAB \\ or\ AABab \end{matrix} \right\}$	$\longrightarrow$	$\left\{ \begin{matrix} (a \sqcup A)b(aa \sqcup A)(B \sqcup b) \\ or\ AAB(AA \sqcup a)(B \sqcup b) \end{matrix} \right\}$
Or	$\left\{ \begin{matrix} (a \sqcup A)Bab \\ or\ aabAB \end{matrix} \right\}$	$\longrightarrow$	$\left\{ \begin{matrix} (a \sqcup A)B(AA \sqcup a)(B \sqcup b) \\ or\ aab(aa \sqcup A)(B \sqcup b) \end{matrix} \right\}$
CFC	3	$\longrightarrow$	$3 \cdot 2$

Table 2.8. Changes Case 1-1 to Case 1-2

These changes make us get the following table from the table of Case 1-1:

All cases	NRT	CFC
CU0	$\binom{k-1}{0}$	$+3^2 2^2 2^{2k-1}\binom{k-1}{0}$
CL0	$\binom{k-1}{0}$	$+3^2 2^2 2^{2k-2}\binom{k-1}{0}$
CU1	$\binom{k-1}{1}$	$-3^2 2^2 2^{2k-3}\binom{k-1}{1}$
CL1	$\binom{k-1}{1}$	$-3^2 2^2 2^{2k-4}\binom{k-1}{1}$
$\vdots$	$\vdots$	$\vdots$
CU(k-2)	$\binom{k-1}{k-2}$	$3^2 2^2 2^3(-1)^{k-2}\binom{k-1}{k-2}$
CL(k-2)	$\binom{k-1}{k-2}$	$3^2 2^2 2^2(-1)^{k-2}\binom{k-1}{k-2}$
CU(k-1)	$\binom{k-1}{k-1}$	$3^2 2^2 2^1(-1)^{k-1}\binom{k-1}{k-1}$
CL(k-1)	$\binom{k-1}{k-1}$	$3^2 2^2(-1)^{k-1}\binom{k-1}{k-1}$

Table 2.9. NRT and CFC of Case 1-2

In addition, the sum of CFC is

$$2^3 3^2[2^{2k-1}\binom{k-1}{0}+2^{2k-2}\binom{k-1}{0}-2^{2k-3}\binom{k-1}{1}-2^{2k-4}\binom{k-1}{1}$$

$$++--\cdots+(-1)^{k-1}2^1\binom{k-1}{k-1}+(-1)^{k-1}2^0\binom{k-1}{k-1}]$$

$$
\begin{aligned}
&= 2^3 3^2 [3\{2^{2k-2}\begin{pmatrix} k-1 \\ 0 \end{pmatrix} - 2^{2k-4}\begin{pmatrix} k-1 \\ 1 \end{pmatrix} + - \cdots + (-1)^{k-1}2^0 \begin{pmatrix} k-1 \\ k-1 \end{pmatrix}\}] \\
&= 2^3 3^3 \{4^{k-1}\begin{pmatrix} k-1 \\ k-1 \end{pmatrix} - 4^{k-2}\begin{pmatrix} k-1 \\ k-2 \end{pmatrix} + - \cdots + (-1)^{k-1}4^0 \begin{pmatrix} k-1 \\ 0 \end{pmatrix}\} \\
&= 2^3 3^3 \sum_{l=0}^{k-1} \begin{pmatrix} k-1 \\ k-1-l \end{pmatrix} 4^{k-1-l}(-1)^l \\
&= 2^3 3^3 3^{k-1} = 2^3 3^{k+2}.
\end{aligned}
$$

Hence the proof of Case 1-2 is completed.

Case 2-1: The coefficients of $a^3b(a^2b)^{2s-1}a^3b^2$ is $3^{s+1}2^2$.

If we compare Case 2-1 and Case 1-1, then we can see that the difference occurs in Part C. Here is the change:

	Case 1-1	Change	Case 2-1
Part C	$\left\{ \begin{matrix} (a \sqcup A)bAB \\ or\ AABab \end{matrix} \right\} a^4b^2$	$\longrightarrow$	$\left\{ \begin{matrix} (a \sqcup A)b(a \sqcup A)B(aa \sqcup A)(B \sqcup b), \\ (a \sqcup A)baab(aa \sqcup A)(B \sqcup b), \\ AAB(A \sqcup a)b(aa \sqcup A)(B \sqcup b), \\ or\ AABAAB(AA \sqcup a)(B \sqcup b) \end{matrix} \right\}$
Or	$\left\{ \begin{matrix} (a \sqcup A)Bab \\ or\ aabAB \end{matrix} \right\} a^4b^2$	$\longrightarrow$	$\left\{ \begin{matrix} (a \sqcup A)B(a \sqcup A)b(A \sqcup aa)(B \sqcup b), \\ (a \sqcup A)BAAB(a \sqcup AA)(B \sqcup b), \\ aab(a \sqcup A)B(AA \sqcup a)(B \sqcup b), \\ or\ aabaab(A \sqcup aa)(b \sqcup B) \end{matrix} \right\}$
CFC	$3^2 2^2$	$\longrightarrow$	$3^2 2$

Table 2.10. Changes Case 1-1 to Case 2-1

If we put s as $k+1$, we can obtain the coefficient of $a^3b(a^2b)^{2s-1}a^3b^2$ as $3^{s+1}2^2$ except for the subcase $s=1$ from Case 1-1.

$a^3ba^2ba^3b^2$ comes for $s=1$ from the following:

$$(aa \sqcup A)b(a \sqcup A)B(a \sqcup AA)(b \sqcup B) \text{ or } (aa \sqcup A)baab(aa \sqcup A)(b \sqcup B).$$

Then, by symmetry, the coefficient is $3^2 2^2$. Thus, we have completed the proof of Case 2-1.

Case 2-2: The coefficient of $a^4bab(a^2b)^{2s-1}ab$ is $3^{s+1}2^2$.

If we compare Case 2-2 and Case 1-2, then we can see that the difference occurs in Part C. Here is the change:

	Case 1-2	Change	Case 2-2
Part C	$\{(a \sqcup A)B(a \sqcup AA)(B \sqcup b)$ or $aab(A \sqcup aa)(B \sqcup b)\}$	$\longrightarrow$	$\{(a \sqcup A)B(a \sqcup A)bAB),$ $(a \sqcup A)BAABab,$ $aab(A \sqcup a)Bab,$ or $aabaabAB\}$
Or	$\{(a \sqcup A)b(A \sqcup aa)(B \sqcup b)$ or $AAB(a \sqcup AA)(B \sqcup b)\}$	$\longrightarrow$	$\{(a \sqcup A)b(a \sqcup A)Bab,$ $(a \sqcup A)baabAB,$ $AAB(a \sqcup A)bAB,$ or $AABAABab\}$
CFC	$3 \cdot 2$	$\longrightarrow$	3

Table 2.11. Changes Case 1-2 to Case 2-2

If we put s as $k+1$, then we can obtain the coefficient of $a^4bab(a^2b)^{2s-1}ab$ as $3^{s+1}2^2$ except for the subcase $s=1$ from the Case 1-2.

a^4baba^2bab comes for $s=1$ from the following:

$$(aa \sqcup AA)baB(a \sqcup A)bAB \text{ or } (aa \sqcup AA)baBAABab.$$

Then, by symmetry , the coefficient of the subcase $s=1$ is $3^2 2^2$. Hence we have completed the proof of Case 2-2.

By the Lemma, we have shown that the only remaining terms on the left hand side are those on the right hand side and the coefficients of every term $\left\{ \begin{array}{c} 2n-1 \\ 2n-j \end{array} \right\}$ are $3^n 2^j$. Hence we complete the proof of Theorem.

2.4.2 Formula from identity 4.

In Theorem 7, if we let $a = \frac{dx}{x}$ and $b = \frac{dx}{1-x}$, then we can get the following results relating nested harmonic sums:

Let us look at the left hand side.

$$\begin{aligned} & \sum_{r=0}^{2n} (-1)^{n-r} [(a^2b)^r \sqcup (a^2b)^{2n-r}] \\ = \quad & (-1)^n \sum_{r=0}^{2n} (-1)^r \int_0^1 \underbrace{\overbrace{a^2b}^{1\ unit} \cdots a^2b}_{r\ units} \int_0^1 \underbrace{a^2b \cdots a^2b}_{2n-r\ units} \\ = \quad & (-1)^n \sum_{r=0}^{2n} \zeta(\{3\}^r; \{1\}^r) \cdot \zeta(\{3\}^{2n-r}; \{1\}^{2n-r}) \end{aligned}$$

by taking integrals over the interval [0,1] and using the definition of nested harmonic sums.

Similarly, we can obtain the right hand side in a the form involving nested harmonic sums if we take an integral over the interval [0,1].

Before giving the formula of the right hand side, we define $\begin{bmatrix} 2n-1 \\ 2n-j \end{bmatrix}$ by $(2n-j)$ transpositions between $'b'$s and their closest $'a'$ on the base

$$\int_0^1 (a^4b^2)^n = \int_0^1 \underbrace{\overbrace{a^4b^2}^{1\ unit}\ a^4b^2 \cdots a^4b^2}_{n\ units}.$$

Then the number of words on $\begin{bmatrix} 2n-1 \\ 2n-j \end{bmatrix}$ is $\begin{pmatrix} 2n-1 \\ 2n-j \end{pmatrix}$.

Let us look at the examples used in the explanation of $\begin{Bmatrix} 2n-1 \\ 2n-j \end{Bmatrix}$.

Example 2.4.2.1. In case $n=3$, $\begin{bmatrix} 5 \\ 1 \end{bmatrix}$ denotes one transposition between ω and its closest Ω on the base $(a^4b^2)^3$, that is,

$$\begin{aligned}
\begin{bmatrix} 5 \\ 1 \end{bmatrix} &= \int_0^1 a^3baba^4b^2a^4b^2 + \int_0^1 a^4baba^3b^2a^4b^2 \\
&+ \int_0^1 a^4b^2a^3baba^4b^2 + \int_0^1 a^4b^2a^4baba^3b^2 \\
&+ \int_0^1 a^4b^2a^4b^2a^3bab \\
&= \zeta(4,2,5,1,5,1;1,1,1,1,1,1) + \zeta(5,2,4,1,5,1;1,1,1,1,1,1) \\
&+ \zeta(5,1,4,2,5,1;1,1,1,1,1,1) + \zeta(5,1,5,2,4,1;1,1,1,1,1,1) \\
&+ \zeta(5,1,5,1,4,2;1,1,1,1,1,1).
\end{aligned}$$

Example 2.4.2.2. Let us look at the case $\begin{bmatrix} 5 \\ 2 \end{bmatrix}$, the number of multiple zeta values is $\begin{pmatrix} 5 \\ 2 \end{pmatrix}$=10 and $\begin{bmatrix} 5 \\ 2 \end{bmatrix}$ denotes two transpositions between bs and their closet a on the base $(a^4b^2)^3$, respectively. That is,

$$\begin{aligned}
\begin{bmatrix} 5 \\ 2 \end{bmatrix} &= \int_0^1 a^3ba^2ba^3b^2a^4b^2 + \int_0^1 a^3baba^3baba^4b^2 \\
&+ \int_0^1 a^3baba^4baba^3b^2 + \int_0^1 a^3baba^4b^2a^3bab \\
&+ \int_0^1 a^4baba^2baba^4b^2 + \int_0^1 a^4baba^3baba^3b^2 \\
&+ \int_0^1 a^4baba^3b^2a^3bab + \int_0^1 a^4b^2a^3ba^2ba^3b^2 \\
&+ \int_0^1 a^4b^2a^3baba^3bab + \int_0^1 a^4b^2a^4baba^2bab \\
&= \zeta(4,3,4,1,5,1;1,1,1,1,1,1) + \zeta(4,2,4,2,5,1;1,1,1,1,1,1) \\
&+ \zeta(4,2,5,2,4,1;1,1,1,1,1,1) + \zeta(4,2,5,1,4,2;1,1,1,1,1,1) \\
&+ \zeta(5,2,3,2,5,1;1,1,1,1,1,1) + \zeta(5,2,4,2,4,1;1,1,1,1,1,1) \\
&+ \zeta(5,2,4,1,4,2;1,1,1,1,1,1) + \zeta(5,1,4,3,4,1;1,1,1,1,1,1) \\
&+ \zeta(5,1,4,2,4,2;1,1,1,1,1,1) + \zeta(5,1,5,2,3,2;1,1,1,1,1,1).
\end{aligned}$$

Hence we get the following formula from Theorem 7:

Formula 8 .

$$\sum_{r=0}^{2n}(-1)^r[\zeta(\{3\}^{n-r};\{1\}^{n-r})\zeta(\{3\}^{n+r};\{1\}^{n+r})] = 3^n\sum_{j=1}^{2n}2^j\begin{bmatrix} 2n-1 \\ 2n-j \end{bmatrix}.$$

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Appendices

Appendix A. Inclusion of multi-sets.

In the following lemmas, we can see the inclusions of multi-sets as the result of the shuffle operation $\sqcup$.

A.1 Inclusion of multi-set 1.

Lemma 6 . *Let S_k be the multi-set of all words as the result of $(a_1 \cdots a_r)^k \sqcup (a_1 \cdots a_r)^{2n-k}$. Then $S_{k-1} \subset S_k$ for $1 \leq k \leq n$.*

Proof. To make the formation of a word in S_k clear, let us put $(a_1 \cdots a_r)^{2n-k}$ as $(A_1 \cdots A_r)^{2n-k}$, then

$$\begin{aligned} S_k &:= \{(a_1 \cdots a_r)^k \sqcup (A_1 \cdots A_r)^{2n-k}\} \\ &= \{a_1 a_2 \cdots a_{rk} \sqcup A_1 A_2 \cdots A_{(2n-k)r}\} \end{aligned}$$

where $a_{j+r} = a_j = A_{j+r} = A_j$ for all $j \geq 1$.

Let $w \in S_{k-1}$. Consider the location of a_1 in the formation of w. If a_1 is located after A_r, then $A_1 \cdots A_r$ can be changed for $a_{r(k-1)+1} \cdots a_{rk}$, which means $w \in S_k$. In addition, the number of choices that $a_1, \cdots, a_{r(k-1)}$ can choose positions at $A_{r+1}, \cdots, A_{r(2n-k+1)}$ is exactly same the number of choices that $a_1, \cdots, a_{r(k-1)}$ can choose positions at $A_1, \cdots, A_{r(2n-k)}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

Suppose a_1 is located before A_r. Consider the location of a_2. If a_2 is located after A_{r+1}, then

$$(A_1 \cdots A_{r-1} \sqcup a_1) A_r A_{r+1}$$

can be changed for

$$(a_{r(k-1)+1}\cdots a_{rk-1}\sqcup A_1)a_{rk}a_1,$$

which means $w\in S_k$. In addition, the number of choices that $a_2,\cdots,a_{r(k-1)}$ can choose positions at $A_{r+2},\cdots,A_{r(2n-k+1)}$ is exactly same the number of choices that $a_2,\cdots,a_{r(k-1)}$ can choose positions at $A_2,\cdots,A_{r(2n-k)}$, which means the multiplicity of $w\in S_{k-1}$ is equal to that of $w\in S_k$.

Assume a_l is located before A_{r+l-1}. If a_{l+1} is located after A_{r+l}, then

$$(a_1\cdots a_l\sqcup A_1\cdots A_{r+l-2})A_{r+l-1}A_{r+l}$$

can be changed for

$$(A_1\cdots A_l\sqcup a_1\cdots a_{r+l-1})a_{r+l-1}a_{r+l},$$

which means $w\in S_k$. In addition, the number of choices that $a_{l+1},\cdots,a_{r(k-1)}$ can choose positions at $A_{r+l},\cdots,A_{r(2n-k+1)}$ is equal to that of choices that $a_{l+1},\cdots,a_{r(k-1)}$ can choose positions at $A_l,\cdots,A_{r(2n-k)}$, which means the multiplicity of $w\in S_{k-1}$ is equal to that of $w\in S_k$.

Assume $a_{r(k-1)-1}$ is located before A_{rk-2}. If $a_{r(k-1)}$ is located after A_{rk-1}, then

$$(a_1\cdots a_{r(k-1)-1}\sqcup A_1\cdots A_{rk-3})A_{rk-2}A_{rk-1}$$

can be changed for

$$(A_1\cdots A_{r(k-1)-1}\sqcup a_1\cdots a_{rk-3})a_{rk-2}a_{rk-1},$$

which means $w\in S_k$. In addition, the number of choices that $a_{r(k-1)}$ can choose positions at $A_{rk-1},\cdots,A_{r(2n-k+1)}$ is equal to that of choices that $a_{r(k-1)}$ can choose positions at $A_{r(k-1)-1},\cdots,A_{r(2n-k)}$, which means the multiplicity of

$w \in S_{k-1}$ is equal to that of $w \in S_k$.

If $a_{r(k-1)}$ is located before A_{rk-1}, then there exists unbroken tail

$$A_{(2n-k)r+1} \cdots A_{(2n-k+1)r},$$

since $k \leq n$. Since

$$u := A_{(2n-k)r+1} \cdots A_{(2n-k+1)r}$$

can be changed for

$$a_{(2n-k)r+1} \cdots a_{(2n-k+1)r},$$

then $w \in S_k$. In addition, the number of occurrences of $w \in S_{k-1}$ is exactly equal to the number of occurrences of $w \in S_k$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$. If we can switch u at other locations after A_{rk-1}, the multiplicity of $w \in S_{k-1}$ is less than that of $w \in S_k$.

•

Hence every words in S_{k-1} is in S_k and its multiplicity is less than or equal to the multiplicity in S_k, which shows that $S_{k-1} \subset S_k$.

A.2 Inclusion of multi-set 2.

Lemma 7 . *Let S_k be the set of all words as the result of $(a_1 \cdots a_r)^k a_1 \cdots a_l \sqcup (a_1 \cdots a_r)^{2n-k} a_1 \cdots a_m$ where $0 \leq l, m \leq r$, $l \leq m$. Then $S_{k-1} \subset S_k$ for $1 \leq k \leq n$.*

Proof. To make the formation of a word in S_k clear, let us put $(a_1 \cdots a_r)^{2n-k}$ $a_1 \cdots a_m$ as $(A_1 \cdots A_r)^{2n-k} A_1 \cdots A_m$, then

$$\begin{aligned} S_k &:= \{(a_1 \cdots a_r)^k a_1 \cdots a_l \sqcup (A_1 \cdots A_r)^{2n-k} A_1 \cdots A_m\} \\ &= \{a_1 a_2 \cdots a_{rk+l} \sqcup A_1 A_2 \cdots A_{(2n-k)r+m}\} \end{aligned}$$

where $a_{j+r} = a_j = A_{j+r} = A_j$ for all $j \geq 1$.

Let $w \in S_{k-1}$. Consider the location of a_1 in the formation of w. If a_1 is located after A_r, then $A_1 \cdots A_r$ can be changed for $a_{r(k-1)+1} \cdots a_{rk}$, which means $w \in S_k$. In addition, the number of choices that $a_1, \cdots, a_{r(k-1)+l}$ can choose positions at $A_{r+1}, \cdots, A_{r(2n-k+1)+m}$ is exactly same the number of choices that $a_1, \cdots, a_{r(k-1)+l}$ can choose positions at $A_1, \cdots, A_{r(2n-k)+m}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

Suppose a_1 is located before A_r. Consider the location of a_2. If a_2 is located after A_{r+1}, then

$$(A_1 \cdots A_{r-1} \sqcup a_1) A_r A_{r+1}$$

can be changed for

$$(a_{r(k-1)+1} \cdots a_{rk-1} \sqcup A_1) a_{rk} a_1,$$

which means $w \in S_k$. In addition, the number of choices that $a_2 \cdots, a_{r(k-1)+l}$ can choose positions at $A_{r+2}, \cdots, A_{r(2n-k+1)+m}$ is exactly same the number of choices that $a_2, \cdots, a_{r(k-1)+l}$ can choose positions at $A_2, \cdots, A_{r(2n-k)+m}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

Assume a_l is located before A_{r+l-1}. If a_{l+1} is located after A_{r+l}, then

$$(a_1 \cdots a_l \sqcup A_1 \cdots A_{r+l-2}) A_{r+l-1} A_{r+l}$$

can be changed for

$$(A_1 \cdots A_l \sqcup a_1 \cdots a_{r+l-1}) a_{r+l-1} a_{r+l},$$

which means $w \in S_k$. In addition, the number of choices that $a_{l+1}, \cdots, a_{r(k-1)+l}$ can choose positions at $A_{r+l}, \cdots, A_{r(2n-k+1)+m}$ is equal to that of choices that

$a_{l+1}, \cdots, a_{r(k-1)+l}$ can choose positions at $A_l, \cdots, A_{r(2n-k)+m}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

Assume $a_{r(k-1)-1+l}$ is located before A_{rk-2+l}. If $a_{r(k-1)+l}$ is located after A_{rk-1+l}, then

$$(a_1 \cdots a_{r(k-1)-1+l} \sqcup A_1 \cdots A_{rk-3+l})A_{rk-2+l}A_{rk-1+l}$$

can be changed for

$$(A_1 \cdots A_{r(k-1)-1+l} \sqcup a_1 \cdots a_{rk-3+l})a_{rk-2+l}a_{rk-1+l},$$

which means $w \in S_k$. In addition, the number of choices that $a_{r(k-1)+l}$ can choose positions at $A_{rk-1+l}, \cdots, A_{r(2n-k+1)+l}$ is equal to that of choices that $a_{r(k-1)+l}$ can choose positions at $A_{r(k-1)-1+l}, \cdots, A_{r(2n-k)+l}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

If $a_{r(k-1)+l}$ is located before A_{rk-1+l}, then there exists unbroken tail

$$A_{(2n-k)r+1+l} \cdots A_{(2n-k+1)r+l} \cdots A_{(2n-k+1)r+m},$$

since $k \leq n$. Since

$$u := A_{(2n-k)r+1+l} \cdots A_{(2n-k+1)r+l}$$

can be changed for

$$a_{(2n-k)r+1+l} \cdots a_{(2n-k+1)r+l},$$

then $w \in S_k$. In addition, the number of occurrences of $w \in S_{k-1}$ is exactly equal to the number of occurrences of $w \in S_k$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$. If we can switch u at other locations after A_{rk-1+l}, the multiplicity of $w \in S_{k-1}$ is less than that of $w \in S_k$.

Hence every words in S_{k-1} is in S_k and its multiplicity is less than or equal to the multiplicity in S_k, which shows that $S_{k-1} \subset S_k$.

A.3 Inclusion of multi-set 3.

Lemma 8 . *Let S_k be the multi-set of all words as the result of $(a_1a_2)^k \sqcup (a_2a_1)^{2n-k}$. Then $S_{k-1} \subset S_k$, for $1 \leq k \leq n$.*

Proof. To make the formation of a word in S_k clear, let's put $(a_2a_1)^{2n-k}$ as $(A_2A_1)^{2n-k}$, then

$$\begin{aligned} S_k : &= \{(a_1a_2)^k \sqcup (a_2a_1)^{2n-k}\} \\ &= \{(a_1a_2\cdots a_{2k}) \sqcup (A_0A_1\cdots A_{2(2n-k)-1})\} \end{aligned}$$

where $a_{j+2} = a_j = A_j = A_{j+2}$ for all $j \geq 1$.

Let $w \in S_{k-1}$. Consider the location of a_1 in the formation of w. If a_1 is located after A_2, then $A_0A_1A_2$ can be changed for $A_0a_{2k-1}a_{2k}$, which means $w \in S_k$. In addition, the number of choices that $a_1, \cdots, a_{2(k-1)}$ can choose positions at $A_3, \cdots, A_{2k-1}$ is exactly same the number of choices that $a_1, \cdots, a_{2(k-1)}$ can choose positions at $A_1, \cdots, A_{2k-3}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

Suppose a_1 is located before A_2. Consider the location of a_2. If a_2 is located after A_3, then

$$(A_0A_1 \sqcup a_1)A_2A_3$$

can be changed for

$$(A_0A_1 \sqcup a_{2k})a_{2k+1}a_1,$$

which means $w \in S_k$. In addition, the number of choices that $a_2, \cdots, a_{2(k-1)}$ can choose positions at $A_4, \cdots, A_{2(2n-k+1)}$ is exactly same the number of choices that $a_2, \cdots, a_{r(k-1)}$ can choose positions at $A_2, \cdots, A_{2(2n-k)}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

Assume a_l is located before A_{l+1}. If a_{l+1} is located after A_{l+2}, then

$$(a_1 \cdots a_l \sqcup A_0 \cdots A_l)A_{l+1}A_{l+2}$$

can be changed for

$$(a_1 \cdots a_l \sqcup A_0 \cdots A_l)a_{2k-1}a_{2k},$$

if l is even

$$(a_1 \cdots a_l \sqcup A_0 \cdots A_l)a_{2k}a_{2k+1},$$

if l is odd, which means $w \in S_k$. In addition, the number of choices that $a_{l+1}, \cdots, a_{2(k-1)}$ can choose positions at $A_{l+2}, \cdots, A_{2(2n-k+1)}$ is equal to that of choices that $a_{l+1}, \cdots, a_{2(k-1)}$ can choose positions at $A_l, \cdots, A_{2(2n-k)}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

Assume $a_{2(k-1)-1}$ is located before A_{2k-2}. If $a_{2(k-1)}$ is located after A_{2k-1}, then

$$(a_1 \cdots a_{2(k-1)-1} \sqcup A_0 \cdots A_{2k-3})A_{2k-2}A_{2k-1}$$

can be changed for

$$(a_1 \cdots a_{2(k-1)-1} \sqcup A_0 \cdots A_{2k-3})a_{2k}a_{2k+1},$$

which means $w \in S_k$. In addition, the number of choices that $a_{2(k-1)}$ can choose positions at $A_{2k-1}, \cdots, A_{2(2n-k+1)}$ is equal to that of choices that $a_{2(k-1)}$ can choose positions at $A_{2(k-1)-1}, \cdots, A_{2(2n-k)}$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$.

If $a_{2(k-1)}$ is located before A_{2k-1}, then there exists unbroken tail

$$A_{2(2n-k)-1}A_{2(2n-k)}A_{2(2n-k)+1},$$

since $k \leq n$. Since

$$u := A_{2(2n-k)-1}A_{2(2n-k)}$$

can be changed for

$$a_{2(2n-k)-1}a_{2(2n-k)},$$

then $w \in S_k$. In addition, the number of occurrences of $w \in S_{k-1}$ is exactly equal to the number of occurrences of $w \in S_k$, which means the multiplicity of $w \in S_{k-1}$ is equal to that of $w \in S_k$. If we can switch u at other locations after A_{2k-1}, the multiplicity of $w \in S_{k-1}$ is less than that of $w \in S_k$.

Hence every words in S_{k-1} is in S_k and its multiplicity is less than or equal to the multiplicity in S_k, which shows that $S_{k-1} \subset S_k$.

Appendix B. Binomial coefficients.

B.1 Binomial coefficient 1.

Lemma 9 . $\sum_{r=0}^{2n}(-1)^{n-r}\begin{pmatrix} 4n \\ 2r \end{pmatrix} = 4^n.$

Proof. Since

$$\begin{aligned}
(1+i)^{4n}+(1-i)^{4n} &= \sum_{k=0}^{4n}\begin{pmatrix} 4n \\ k \end{pmatrix} i^k + \sum_{k=0}^{4n}\begin{pmatrix} 4n \\ k \end{pmatrix}(-i)^k \\
&= \sum_{r=0}^{2n}\begin{pmatrix} 4n \\ 2r \end{pmatrix}(-1)^r + \sum_{r=0}^{2n}\begin{pmatrix} 4n \\ 2r \end{pmatrix}(-1)^r \\
&= 2\sum_{r=0}^{2n}\begin{pmatrix} 4n \\ 2r \end{pmatrix}(-1)^r,
\end{aligned}$$

then

$$\begin{aligned}
\sum_{r=0}^{2n}(-1)^{n-r}\begin{pmatrix} 4n \\ 2r \end{pmatrix} &= \frac{(-1)^n}{2}\{(1+i)^{4n}+(1-i)^{4n}\} \\
&= \frac{(-1)^n}{2}\{(-4)^n+(-4)^n\} \\
&= 4^n.
\end{aligned}$$

B.2 Binomial coefficient 2.

Lemma 10 . $\sum_{r=0}^{2n}(-1)^{n-r}\begin{pmatrix} 4n+1 \\ 2r+1 \end{pmatrix} = 4^n.$

Proof. Since

$$
\begin{aligned}
(1+i)^{4n+1}-(1-i)^{4n+1} &= \sum_{k=0}^{4n+1}\begin{pmatrix}4n+1\\k\end{pmatrix} i^k - \sum_{k=0}^{4n+1}\begin{pmatrix}4n+1\\k\end{pmatrix}(-i)^k \\
&= \sum_{r=0}^{2n}\begin{pmatrix}4n+1\\2r+1\end{pmatrix} i^{2r+1} + \sum_{r=0}^{2n}\begin{pmatrix}4n+1\\2r+1\end{pmatrix} i^{2r+1} \\
&= 2i\sum_{r=0}^{2n}\begin{pmatrix}4n+1\\2r+1\end{pmatrix}(-1)^r,
\end{aligned}
$$

then

$$
\begin{aligned}
\sum_{r=0}^{2n}(-1)^{n-r}\begin{pmatrix}4n+1\\2r+1\end{pmatrix} &= \frac{(-1)^n}{2i}\{(1+i)^{4n+1}-(1-i)^{4n+1}\} \\
&= \frac{(-1)^n}{2i}\{(-4)^n(1+i)-(-4)^n(1-i)\} \\
&= 4^n.
\end{aligned}
$$

B.3 Binomial coefficient 3.

Lemma 11 . $\sum_{r=0}^{2n}(-1)^{n-r}\begin{pmatrix}4n+2\\2r+1\end{pmatrix} = 2\cdot 4^n.$

Proof. Since

$$
\begin{aligned}
(1+i)^{4n+2}-(1-i)^{4n+2} &= \sum_{k=0}^{4n+2}\begin{pmatrix}4n+2\\k\end{pmatrix} i^k - \sum_{k=0}^{4n+2}\begin{pmatrix}4n+2\\k\end{pmatrix}(-i)^k \\
&= \sum_{r=0}^{2n}\begin{pmatrix}4n+2\\2r+1\end{pmatrix} i^{2r+1} + \sum_{r=0}^{2n}\begin{pmatrix}4n+2\\2r+1\end{pmatrix} i^{2r+1} \\
&= 2i\sum_{r=0}^{2n}\begin{pmatrix}4n+1\\2r+1\end{pmatrix}(-1)^r,
\end{aligned}
$$

then

$$
\begin{aligned}
\sum_{r=0}^{2n}(-1)^{n-r}\begin{pmatrix}4n+2\\2r+1\end{pmatrix} &= \frac{(-1)^n}{2i}\{(1+i)^{4n+2}-(1-i)^{4n+2}\}\\
&= \frac{(-1)^n}{2i}\{(-4)^n 2i+(-4)^n 2i\}\\
&= 2\cdot 4^n.
\end{aligned}
$$

B.4 Binomial coefficient 4.

Lemma 12 . $\sum_{r=0}^{2n+1}(-1)^{n-r}\begin{pmatrix}4n+3\\2r+1\end{pmatrix}=2\cdot 4^n$.

Proof. Since

$$
\begin{aligned}
(1+i)^{4n+3}-(1-i)^{4n+3} &= \sum_{k=0}^{4n+3}\begin{pmatrix}4n+3\\k\end{pmatrix}i^k-\sum_{k=0}^{4n+3}\begin{pmatrix}4n+3\\k\end{pmatrix}(-i)^k\\
&= \sum_{r=0}^{2n+1}\begin{pmatrix}4n+3\\2r+1\end{pmatrix}i^{2r+1}+\sum_{r=0}^{2n+1}\begin{pmatrix}4n+3\\2r+1\end{pmatrix}i^{2r+1}\\
&= 2i\sum_{r=0}^{2n+1}\begin{pmatrix}4n+3\\2r+1\end{pmatrix}(-1)^r,
\end{aligned}
$$

then

$$
\begin{aligned}
\sum_{r=0}^{2n+1}(-1)^{n-r}\begin{pmatrix}4n+3\\2r+1\end{pmatrix} &= \frac{(-1)^n}{2i}\{(1+i)^{4n+3}-(1-i)^{4n+3}\}\\
&= \frac{(-1)^n}{2i}\{(-4)^n(1+i)2i+(-4)^n(1-i)2i\}\\
&= 2\cdot 4^n.
\end{aligned}
$$

B.5 Binomial coefficient 5.

Lemma 13 .

$$\sum_{k=0}^{2n}(-1)^{n-k}\begin{pmatrix} 6n \\ 3r \end{pmatrix} = 3^n\sum_{j=1}^{2n}2^j\begin{pmatrix} 2n-1 \\ 2n-j \end{pmatrix} = 2\cdot 3^{3n-1}.$$

Proof. By the binomial theorem, we get the following:

$$(-1)^n 3^{3n} = (1-\omega)^{6n} = \sum_{j=0}^{6n}(-1)^j\begin{pmatrix} 6n \\ j \end{pmatrix}\omega^j$$

$$(-1)^n 3^{3n} = (1-\overline{\omega})^{6n} = \sum_{j=0}^{6n}(-1)^j\begin{pmatrix} 6n \\ j \end{pmatrix}\overline{\omega}^j$$

$$0 = (1-1)^{6n} = \sum_{j=0}^{6n}(-1)^j\begin{pmatrix} 6n \\ j \end{pmatrix}$$

where $\omega = \cos(\frac{2\pi}{3}) + i\sin(\frac{2\pi}{3})$.

From these equations, we can obtain the following:

$$2(-1)^n 3^{3n} = 3\sum_{j=0}^{2n}(-1)^j\begin{pmatrix} 6n \\ 3j \end{pmatrix}.$$

Hence

$$\begin{aligned}(RHS) &= 3^n\sum_{j=1}^{2n}2^j\begin{pmatrix} 2n-1 \\ 2n-j \end{pmatrix} \\ &= 3^n\sum_{j=1}^{2n}2^j\begin{pmatrix} 2n-1 \\ j-1 \end{pmatrix} \\ &= 3^n\sum_{j=0}^{2n-1}2^{j+1}\begin{pmatrix} 2n-1 \\ j \end{pmatrix}\end{aligned}$$

$$
\begin{aligned}
&= 3^n 2 \sum_{j=0}^{2n-1} 2^j \begin{pmatrix} 2n-1 \\ j \end{pmatrix} \\
&= 2 \cdot 3^{3n-1} \\
&= (-1)^n \sum_{j=0}^{2n} (-1)^j \begin{pmatrix} 6n \\ 3j \end{pmatrix} = (LHS).
\end{aligned}
$$

BIOGRAPHY OF THE AUTHOR

Ji Hoon Ryoo was born in Milyang, Rep. of Korea on April 23, 1972. He was raised in Pusan, Rep. of Korea and graduated from Pusan Sajik High School in 1991. He attended Kyungpook National University from the spring of 1992. From 1993 to 1994, he had served in army. From 1994 to 1995, he had worked as an assistant instructor at private institutes in Pusan, Rep. of Korea. He graduated from Kyungpook National University in 1999 with a Bachelor's degree in Mathematics. He entered The graduate program in mathematics and statistics at The University of Maine in the fall of 1999.

After receiving his degree, Ji Hoon will continue in Ph.D program at The University of Minnesota, Twin Cities. Ji Hoon is a candidate for the Master of Arts degree in Mathematics from The University of Maine in May, 2001.