TAIWANESE JOURNAL OF MATHEMATICS
Vol. 20, No. 2, pp. 243–261, April 2016
DOI: 10.11650/tjm.20.2016.5487
This paper is available online at http://journal.tms.org.tw

On Vectorized Weighted Sum Formulas of Multiple Zeta Values

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Abstract. In this paper, we introduce the vectorization of shuffle products of two sums of multiple zeta values, which generalizes the weighted sum formula obtained by Ohno and Zudilin. Some interesting weighted sum formulas of vectorized type are obtained, such as

$$\begin{aligned}&\sum_{\substack{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}\\ |\boldsymbol{\alpha}|:\text{even}}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) \sum_{|\boldsymbol{c}|=|\boldsymbol{k}|+r+3} 2^{c_{|\boldsymbol{\alpha}|+1}}\zeta(c_0,c_1,\dots,c_{|\boldsymbol{\alpha}|},\dots,c_{|\boldsymbol{k}|+1}+1)\\ &= \frac{1}{2}(2|\boldsymbol{k}|+r+5)M(\boldsymbol{k})\zeta(|\boldsymbol{k}|+r+4),\end{aligned}$$

where $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ and $\boldsymbol{k}$ are n-tuples of nonnegative integers with $|\boldsymbol{k}| = k_1+k_2+\cdots+k_n$ even; $M(\boldsymbol{u})$ is the multinomial coefficient defined by $\binom{u_1+u_2+\cdots+u_n}{u_1,u_2,\dots,u_n}$ with the value $\frac{|\boldsymbol{u}|!}{u_1!u_2!\cdots u_n!}$; and r is a nonnegative integer. Moreover, some newly developed combinatorial identities of vectorized types involving multinomial coefficients by extending the shuffle products of two sums of multiple zeta values in their vectorizations are given as well.

1. Introduction and statements of results

A *multiple zeta value* (see e.g. [1, p. 189]) is defined for a string $\boldsymbol{\alpha} = (\alpha_1,\alpha_2,\dots,\alpha_r)$ of positive integers with $\alpha_r \geq 2$ by a convergent series

$$\zeta(\boldsymbol{\alpha}) = \zeta(\alpha_1,\alpha_2,\dots,\alpha_r) := \sum_{1\leq n_1<n_2<\cdots<n_r} n_1^{-\alpha_1}n_2^{-\alpha_2}\cdots n_r^{-\alpha_r}. \tag{1.1}$$

The numbers $|\boldsymbol{\alpha}| = \alpha_1+\alpha_2+\cdots+\alpha_r$ and r are called the *weight* and *depth* of $\zeta(\boldsymbol{\alpha})$, respectively.

For convenience, we let $\{1\}^k$ be k repetitions of 1. For example,

$$\zeta(\{1\}^2, 3) = \zeta(1,1,3) \quad\text{and}\quad \zeta(2,\{1\}^4, 5) = \zeta(2,1,1,1,1,5).$$

Received October 24, 2014, accepted September 20, 2015.
Communicated by Yu-Ru Liu.
2010 *Mathematics Subject Classification*. Primary: 40A25, 40B05; Secondary: 11M41, 11M06, 33E20.
Key words and phrases. Multiple zeta value, Shuffle relation, Sum formula, Weighted sum formula.
Chung thanks the support of Institute of Mathematics, Academia Sinica, Taiwan.
Ong was supported by the Ministry of Science and Technology of Taiwan.
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The following two formulas are well known. The first is the celebrated sum formula (see [6, p. 95] or [2, p. 74]) and the second is a weighted sum formula of Y. Ohno and W. Zudilin [7, p. 329]:

$$\sum_{|\boldsymbol{\alpha}|=m} \zeta(\alpha_1, \dots, \alpha_{r-1}, \alpha_r + 1) = \zeta(m+1), \tag{1.2}$$

$$\sum_{|\boldsymbol{\alpha}|=m} 2^{\alpha_2} \zeta(\alpha_1, \alpha_2 + 1) = \frac{1}{2}(m+2)\zeta(m+1), \tag{1.3}$$

for any positive integers $m \geq r$. Hereafter we restrict all variables $\alpha_1, \alpha_2, \dots, \alpha_r$ appearing in a multiple zeta value to be positive integers.

There is an integral representation, due to Kontsevich (see e.g. [9, p. 510]) for multiple zeta values in terms of iterated integrals (or Drinfel'd integrals) as a weight-dimensional integral:

$$\zeta(\boldsymbol{\alpha}) = \int_I \Omega_1 \Omega_2 \cdots \Omega_{|\boldsymbol{\alpha}|} = \int_0^1 \cdots \left(\int_0^{t_3} \left(\int_0^{t_2} \Omega_1 \right) \Omega_2 \right) \cdots \Omega_{|\boldsymbol{\alpha}|}, \tag{1.4}$$

where the integral is taken over the simplex $I : 0 < t_1 < t_2 < \cdots < t_{|\boldsymbol{\alpha}|} < 1$, the differential 1-forms $\Omega_j = dt_j/(1-t_j)$ if $j \in \{1, \alpha_1 + 1, \alpha_1 + \alpha_2 + 1, \dots, \alpha_1 + \alpha_2 + \cdots + \alpha_{r-1} + 1\}$ and $\Omega_j = dt_j/t_j$ otherwise. An elementary consideration yields a depth-dimensional integral representation as

$$\begin{aligned} &\zeta(\alpha_1, \dots, \alpha_{r-1}, \alpha_r + 1) \\ &= \frac{1}{(\alpha_1 - 1)! \cdots (\alpha_{r-1} - 1)! \alpha_r!} \int_{0<t_1<t_2<\cdots<t_r<1} \frac{dt_1}{1-t_1} \left(\log \frac{t_2}{t_1} \right)^{\alpha_1 - 1} \\ &\qquad \times \frac{dt_2}{1-t_2} \left(\log \frac{t_3}{t_2} \right)^{\alpha_2 - 1} \cdots \frac{dt_r}{1-t_r} \left(\log \frac{1}{t_r} \right)^{\alpha_r}. \end{aligned} \tag{1.5}$$

In particular, for positive integers m and n, we have

$$\zeta(\{1\}^{m-1}, n+1) = \int_{0<t_1<t_2<\cdots<t_{m+n}<1} \prod_{j=1}^{m} \frac{dt_j}{1-t_j} \prod_{k=m+1}^{m+n} \frac{dt_k}{t_k}, \tag{1.6}$$

from which the so-called Drinfel'd duality theorem [9, p. 510] follows easily:

$$\zeta(\{1\}^{m-1}, n+1) = \zeta(\{1\}^{n-1}, m+1). \tag{1.7}$$

It is worth to note that we are able to express the product of two sums of multiple zeta values as a linear combination of multiple zeta values through the shuffle product of sums of multiple zeta values by their Drinfel'd integral representations.

The shuffle product of two multiple zeta values is defined as

$$\int \Omega_1\Omega_2\cdots\Omega_m \int \Omega_{m+1}\Omega_{m+2}\cdots\Omega_{m+n} = \sum_{\sigma} \int \Omega_{\sigma(1)}\Omega_{\sigma(2)}\cdots\Omega_{\sigma(m+n)}, \tag{1.8}$$

where the sum is taken over all $\binom{m+n}{m}$ permutations σ of the set $\{1,2,\ldots,m+n\}$, which preserve the orders of strings of differential forms $\Omega_1\Omega_2\cdots\Omega_m$ and $\Omega_{m+1}\Omega_{m+2}\cdots\Omega_{m+n}$. More precisely, the permutation σ satisfies the condition

$$\sigma^{-1}(i) < \sigma^{-1}(j)$$

for all $1 \le i < j \le m$ and $m+1 \le i < j \le m+n$. Unfortunately, it is typically painful and laborious to produce shuffle relations from shuffle products. We, therefore, restrict our attention to the so-called height-one multiple zeta value

$$\zeta(\{1\}^{m-1}, n+1),$$

or sums of multiple zeta values which can be further expressed as integrals (in one variable) or double integrals (in two variables).

The following two propositions are essential to transform multiple zeta values into integrals, and vice versa.

Proposition 1.1. [3,4] *For nonnegative integers m and n, we have*

$$\begin{aligned} \zeta(\{1\}^m, n+2) &= \frac{1}{m!(n+1)!}\int_0^1 \left(\log\frac{1}{1-t}\right)^m \left(\log\frac{1}{t}\right)^{n+1} \frac{dt}{1-t} \\ &= \frac{1}{m!n!}\int_{0<t_1<t_2<1} \left(\log\frac{1}{1-t_1}\right)^m \left(\log\frac{1}{t_2}\right)^n \frac{dt_1dt_2}{(1-t_1)t_2}. \end{aligned} \tag{1.9}$$

Proposition 1.2. [3,4] *For nonnegative integers p,q,r and n, we have*

$$\begin{aligned} &\sum_{|\boldsymbol{\alpha}|=q+r+1} \zeta(\{1\}^p, \alpha_0,\ldots,\alpha_{q-1},\alpha_q+n+1) \\ &= \frac{1}{p!q!r!n!}\int_{0<t_1<t_2<1} \left(\log\frac{1}{1-t_1}\right)^p \left(\log\frac{1-t_1}{1-t_2}\right)^q \left(\log\frac{t_2}{t_1}\right)^r \left(\log\frac{1}{t_2}\right)^n \frac{dt_1dt_2}{(1-t_1)t_2}. \end{aligned} \tag{1.10}$$

Some generalizations of the weighted sum formula has already been given. For example, the integral

$$\frac{1}{k!r!}\iint_{R_1\times R_2} \left(\log\frac{1-t_1}{1-t_2} - \log\frac{1-u_1}{1-u_2}\right)^k \left(\log\frac{t_2}{t_1} + \log\frac{u_2}{u_1}\right)^r \frac{dt_1dt_2}{(1-t_1)t_2}\frac{du_1du_2}{(1-u_1)u_2} \tag{1.11}$$

with $R_1: 0<t_1<t_2<1$, $R_2: 0<u_1<u_2<1$; and a pair of nonnegative integers k,r with k even, leads to the following.

Theorem 1.3. [8, p. 1189] *For a pair of positive integers m and k with $m \geq k$, we have*

$$\sum_{|\boldsymbol{\alpha}|=m} \sum_{\substack{j=1,\\ j:\text{even}}}^{k} 2^{\alpha_j} \zeta(\alpha_1, \ldots, \alpha_{k-1}, \alpha_k + 1) = \frac{m+k}{2} \zeta(m+1). \tag{1.12}$$

On the other hand, to deal with the case when k is odd, the integral with a parameter μ as

(1.13)

$$\frac{1}{k!r!} \iint_{R_1 \times R_2} \left(\mu \log \frac{1-t_1}{1-t_2} + \log \frac{1-u_1}{1-u_2} \right)^k \left(\log \frac{t_2}{t_1} + \log \frac{u_2}{u_1} \right)^r \frac{dt_1 dt_2}{(1-t_1)t_2} \frac{du_1 du_2}{(1-u_1)u_2}$$

leads to the following.

Theorem 1.4. [8, pp. 1195–1196] *For a pair of positive integers n, k with k odd and $n > k \geq 3$, we have*

$$\begin{aligned} &(k-2) \sum_{\substack{j=2,\\ j:\text{even}}}^{k} \sum_{|\boldsymbol{\alpha}|=n} 2^{\alpha_j} \zeta(\alpha_1, \ldots, \alpha_{k-1}, \alpha_k + 1) \\ &\quad + \sum_{j=1}^{k} (j-1)(-1)^j \sum_{|\boldsymbol{\alpha}|=n} 2^{\alpha_j} \zeta(\alpha_1, \ldots, \alpha_{k-1}, \alpha_k + 1) \\ &\quad + \sum_{\substack{j=2,\\ j:\text{even}}}^{k} \sum_{|\boldsymbol{\alpha}|=n} 2^{\alpha_j} (2^{\alpha_{j+1}} - 2) \zeta(\alpha_1, \ldots, \alpha_{k-1}, \alpha_k + 1) \\ &= \frac{(k-1)(n+k-2)}{2} \zeta(n+1). \end{aligned} \tag{1.14}$$

In this paper, a general procedure of the vectorization of the relations among multiple zeta values, such as the weighted sum formula, is completely developed. We obtain the vectorized weighted sum formula in Sections 2 and 3 simply by changing the specific exponent of the integrand of the integral such as (1.13) into a vector. Finally, several applications of the shuffle relations for two families of multiple zeta values in the combinatorial identities involving multinomial coefficients will be given in the final section.

2. Vectorized weighted sum formulas

Let $R_1 : 0 < t_1 < t_2 < 1$ and $R_2 : 0 < u_1 < u_2 < 1$. For an n-tuple of nonnegative integers $\boldsymbol{k} = (k_1, k_2, \ldots, k_n)$ and another nonnegative integer r, we consider the integral with parameters $\mu_1, \mu_2, \ldots, \mu_n$ given by

$$\begin{aligned} &\frac{1}{k_1! k_2! \cdots k_n! r!} \iint_{R_1 \times R_2} \prod_{i=1}^{n} \left(\mu_i \log \frac{1-t_1}{1-t_2} + \log \frac{1-u_1}{1-u_2} \right)^{k_i} \\ &\qquad \times \left(\log \frac{t_2}{t_1} + \log \frac{u_2}{u_1} \right)^r \frac{dt_1 dt_2}{(1-t_1)t_2} \frac{du_1 du_2}{(1-u_1)u_2}. \end{aligned} \tag{2.1}$$

For convenience, we employ some vectorized notations

$$\boldsymbol{\mu}^{\boldsymbol{\alpha}} = \mu_1^{\alpha_1}\mu_2^{\alpha_2}\cdots\mu_n^{\alpha_n}; \quad \boldsymbol{k}! = k_1!k_2!\cdots k_n!; \quad \boldsymbol{k}+1 = (k_1+1, k_2+1, \ldots, k_n+1)$$

and the multinomial coefficient

$$M(\boldsymbol{\alpha}) = \binom{\alpha_1+\alpha_2+\cdots+\alpha_n}{\alpha_1,\alpha_2,\ldots,\alpha_n} = \frac{|\boldsymbol{\alpha}|!}{\alpha_1!\alpha_2!\cdots\alpha_n!}$$

for an n-tuple of nonnegative integers $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ with $|\boldsymbol{\alpha}| = \alpha_1+\alpha_2+\cdots+\alpha_n$.

If we replace each component

$$\left(\mu_i \log\frac{1-t_1}{1-t_2} + \log\frac{1-u_1}{1-u_2}\right)^{k_i}$$

and

$$\left(\log\frac{t_2}{t_1} + \log\frac{u_2}{u_1}\right)^{r}$$

of the integrand of the integral (2.1) by their binomial expansions as

$$\sum_{\alpha_i+\beta_i=k_i} \frac{k_i!}{\alpha_i!\beta_i!}\mu_i^{\alpha_i}\left(\log\frac{1-t_1}{1-t_2}\right)^{\alpha_i}\left(\log\frac{1-u_1}{1-u_2}\right)^{\beta_i}, \tag{2.2}$$

for $i = 1, 2, \ldots, n$, and

$$\sum_{\ell=0}^{r}\binom{r}{\ell}\left(\log\frac{t_2}{t_1}\right)^{r-\ell}\left(\log\frac{u_2}{u_1}\right)^{\ell}, \tag{2.3}$$

respectively, then the value of the integral (2.1) is given by

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}} \boldsymbol{\mu}^{\boldsymbol{\alpha}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta})\sum_{\ell=0}^{r}\zeta(|\boldsymbol{\alpha}|+r-\ell+2)\zeta(|\boldsymbol{\beta}|+\ell+2) \tag{2.4}$$

in light of Proposition 1.2 and the sum formula (1.2). On the other hand, the domain $R_1 \times R_2$ of the integral is decomposed into six simplices produced from all possible interlacings of variables t_1, t_2, u_1, u_2 in the following:

$$\begin{aligned}
&D_1: \ 0 < t_1 < t_2 < u_1 < u_2 < 1, \quad && D_2: \ 0 < u_1 < u_2 < t_1 < t_2 < 1,\\
&D_3: \ 0 < t_1 < u_1 < t_2 < u_2 < 1, \quad && D_4: \ 0 < t_1 < u_1 < u_2 < t_2 < 1,\\
&D_5: \ 0 < u_1 < t_1 < u_2 < t_2 < 1, \quad && D_6: \ 0 < u_1 < t_1 < t_2 < u_2 < 1.
\end{aligned}$$

For the simplex D_1, substituting the integrands $\left(\mu_i \log\frac{1-t_1}{1-t_2} + \log\frac{1-u_1}{1-u_2}\right)^{k_i}$ and $\left(\log\frac{t_2}{t_1} + \log\frac{u_2}{u_1}\right)^{r}$ by their binomial expansions as (2.2) and (2.3), respectively. Then the value of the integral (2.1) over D_1 in terms of multiple zeta values leads to

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}} \boldsymbol{\mu}^{\boldsymbol{\alpha}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta})\sum_{\ell=0}^{r}\zeta(|\boldsymbol{\alpha}|+r-\ell+2, |\boldsymbol{\beta}|+\ell+2).$$

Similarly, the value of the integral (2.1) over D_2 in terms of multiple zeta values is given by

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}} \boldsymbol{\mu}^{\boldsymbol{\alpha}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) \sum_{\ell=0}^{r} \zeta(|\boldsymbol{\beta}|+\ell+2, |\boldsymbol{\alpha}|+r-\ell+2).$$

Hence, the the total value of the integral (2.1) minus the values of the integrals over D_1 and D_2 is

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}} \boldsymbol{\mu}^{\boldsymbol{\alpha}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta})(r+1)\zeta(|\boldsymbol{k}|+r+4),$$

in light of (2.2) and the reflection formula [5, p. 71]:

$$\zeta(p,q)+\zeta(q,p)=\zeta(p)\zeta(q)-\zeta(p+q), \quad p,q \geq 2.$$

For the simplex D_3, substituting the integrands $\left(\mu_i \log \frac{1-t_1}{1-t_2} + \log \frac{1-u_1}{1-u_2}\right)^{k_i}$ and $\left(\log \frac{t_2}{t_1} + \log \frac{u_2}{u_1}\right)^r$ by their multinomial expansions as

$$\sum_{\alpha_i+\beta_i+\gamma_i=k_i} \mu_i^{\alpha_i}(\mu_i+1)^{\beta_i} \frac{k_i!}{\alpha_i!\beta_i!\gamma_i!} \left(\log \frac{1-t_1}{1-u_1}\right)^{\alpha_i} \left(\log \frac{1-u_1}{1-t_2}\right)^{\beta_i} \left(\log \frac{1-t_2}{1-u_2}\right)^{\gamma_i},$$

and

$$\sum_{m+n+p=r} 2^n \frac{r!}{m!n!p!} \left(\log \frac{u_1}{t_1}\right)^m \left(\log \frac{t_2}{u_1}\right)^n \left(\log \frac{u_2}{t_2}\right)^p,$$

respectively. Then the value of the integral (2.1) over D_3 turns out to be

$$\begin{aligned} &\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}=\boldsymbol{k}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta})M(\boldsymbol{\gamma}) \\ &\quad \times \sum_{m+n+p=r} 2^n \sum_{\substack{|\boldsymbol{c}|=|\boldsymbol{\alpha}|+m+1 \\ |\boldsymbol{d}|=|\boldsymbol{\beta}|+n+1 \\ |\boldsymbol{g}|=|\boldsymbol{\gamma}|+p+1}} \zeta(c_0,c_1,\dots,c_{|\boldsymbol{\alpha}|}, d_0,d_1,\dots,d_{|\boldsymbol{\beta}|}+g_0,g_1,\dots,g_{|\boldsymbol{\gamma}|}+1) \\ &\qquad \times \boldsymbol{\mu}^{\boldsymbol{\alpha}}(\boldsymbol{\mu}+1)^{\boldsymbol{\beta}}. \end{aligned}$$

In the similar manner, we evaluate the values of the integral (2.1) over D_4, D_5 and D_6. Then by adding together all these values of the integrals from D_3 to D_6, we obtain the following shuffle relation:

$$\begin{aligned} &\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}=\boldsymbol{k}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta})M(\boldsymbol{\gamma}) \sum_{m+n+p=r} 2^n \\ &\quad \times \sum_{\substack{|\boldsymbol{c}|=|\boldsymbol{\alpha}|+m+1 \\ |\boldsymbol{d}|=|\boldsymbol{\beta}|+n+1 \\ |\boldsymbol{g}|=|\boldsymbol{\gamma}|+p+1}} \zeta(c_0,c_1,\dots,c_{|\boldsymbol{\alpha}|}, d_0,d_1,\dots,d_{|\boldsymbol{\beta}|}+g_0,g_1,\dots,g_{|\boldsymbol{\gamma}|}+1) \\ &\qquad \times \left[(\boldsymbol{\mu}+1)^{\boldsymbol{\beta}}(\boldsymbol{\mu}^{\boldsymbol{\alpha}}+\boldsymbol{\mu}^{\boldsymbol{\gamma}}+\boldsymbol{\mu}^{\boldsymbol{\alpha}+\boldsymbol{\gamma}}+1)\right] \\ &= \sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}} \boldsymbol{\mu}^{\boldsymbol{\alpha}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta})(r+1)\zeta(|\boldsymbol{k}|+r+4). \end{aligned} \tag{2.5}$$

When $|\boldsymbol{k}|$ is even, setting $\mu_1 = \mu_2 = \cdots = \mu_n = -1$ in (2.5) leads to the following shuffle relation

$$\sum_{\substack{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}\\ |\boldsymbol{\alpha}|:\text{even}}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) \sum_{|\boldsymbol{c}|=|\boldsymbol{k}|+r+3} (2^{c_{|\boldsymbol{\alpha}|+1}}-2)\zeta(c_0,\ldots,c_{|\boldsymbol{k}|},c_{|\boldsymbol{k}|+1}+1) = \frac{1}{2}M(\boldsymbol{k})(r+1)\zeta(|\boldsymbol{k}|+r+4). \tag{2.6}$$

In light of the sum formula

$$\sum_{|\boldsymbol{c}|=|\boldsymbol{k}|+r+3} \zeta(c_0,\ldots,c_{|\boldsymbol{k}|},c_{|\boldsymbol{k}|+1}+1) = \zeta(|\boldsymbol{k}|+r+4)$$

and the identity

$$\begin{aligned} 2\sum_{\substack{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}\\ |\boldsymbol{\alpha}|:\text{even}}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) &= \sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}} \left\{1+(-1)^{|\boldsymbol{\alpha}|}\right\} M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) \\ &= (|\boldsymbol{k}|+2)M(\boldsymbol{k}), \end{aligned}$$

the shuffle relation (2.6) could be rewritten as follows.

Main Theorem 2.1. *Suppose that $\boldsymbol{k} = (k_1, k_2, \ldots, k_n)$ is an n-tuple of nonnegative integers and r is a nonnegative integer. When $|\boldsymbol{k}| = k_1 + k_2 + \cdots + k_n$ is even, we have*

$$\begin{aligned} &\sum_{\substack{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}\\ |\boldsymbol{\alpha}|:\text{even}}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) \sum_{|\boldsymbol{c}|=|\boldsymbol{k}|+r+3} 2^{c_{|\boldsymbol{\alpha}|+1}}\zeta(c_0,\ldots,c_{|\boldsymbol{\alpha}|},\ldots,c_{|\boldsymbol{k}|},c_{|\boldsymbol{k}|+1}+1) \\ &= \frac{1}{2}(2|\boldsymbol{k}|+r+5)M(\boldsymbol{k})\zeta(|\boldsymbol{k}|+r+4). \end{aligned}$$

When $|\boldsymbol{k}|$ is odd, then at least one of $k_1, k_2, \ldots, k_n$ should be odd. Without lost of generality, we suppose that k_1 is odd. Multiply both sides of (2.5) by μ_1 and then differentiate (2.5) with respect to μ_1. Setting $\mu_1 = \mu_2 = \cdots = \mu_n = -1$ leads to the following.

Theorem 2.2. *Suppose that $\boldsymbol{k} = (k_1, k_2, \ldots, k_n)$ is an n-tuple of nonnegative integers with both $|\boldsymbol{k}|$ and k_1 odd, and r is a nonnegative integer. Then we have*

$$\begin{aligned} &k_1 \sum_{\substack{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}\\ |\boldsymbol{\alpha}|:\text{even}}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) \sum_{|\boldsymbol{c}|=|\boldsymbol{k}|+r+3} (2^{c_{|\boldsymbol{\alpha}|+1}}-2)\zeta(c_0,\ldots,c_{|\boldsymbol{\alpha}|},\ldots,c_{|\boldsymbol{k}|},c_{|\boldsymbol{k}|+1}+1) \\ &+ \sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}} \alpha_1(-1)^{|\boldsymbol{\alpha}|}M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) \sum_{|\boldsymbol{c}|=|\boldsymbol{k}|+r+3} (2^{c_{|\boldsymbol{\alpha}|+1}}-2)\zeta(c_0,\ldots,c_{|\boldsymbol{\alpha}|},\ldots,c_{|\boldsymbol{k}|},c_{|\boldsymbol{k}|+1}+1) \\ &+ \sum_{\substack{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}\\ |\boldsymbol{\alpha}|:\text{even}\\ \alpha_1\le k_1-1}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta}) \sum_{|\boldsymbol{c}|=|\boldsymbol{k}|+r+3} 2^{c_{|\boldsymbol{\alpha}|+1}}(2^{c_{|\boldsymbol{\alpha}|+2}}-2)\zeta(c_0,\ldots,c_{|\boldsymbol{\alpha}|},\ldots,c_{|\boldsymbol{k}|},c_{|\boldsymbol{k}|+1}+1) \\ &= \sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}} (\alpha_1+1)(-1)^{|\boldsymbol{\alpha}|+1}M(\boldsymbol{\alpha})M(\boldsymbol{\beta})(r+1)\zeta(|\boldsymbol{k}|+r+4). \end{aligned}$$

Also if we set $\mu_1 = \mu_2 = \cdots = \mu_n = 1$ in (2.5), then we obtain another vectorized shuffle relation in the following.

Theorem 2.3. *Suppose that $\boldsymbol{k} = (k_1, k_2, \ldots, k_n)$ is an n-tuple of nonnegative integers and r is a nonnegative integer. Then*

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}=\boldsymbol{k}} M(\boldsymbol{\alpha})M(\boldsymbol{\beta})M(\boldsymbol{\gamma}) \sum_{|\boldsymbol{c}|=|\boldsymbol{k}|+r+3} w(|\boldsymbol{\alpha}|, |\boldsymbol{\beta}|)\zeta(c_0, \ldots, c_{|\boldsymbol{\alpha}|}, \ldots, c_{|\boldsymbol{k}|}, c_{|\boldsymbol{k}|+1} + 1)$$
$$= \frac{1}{2}(|\boldsymbol{k}| + 1)(r + 1)M(\boldsymbol{k})\zeta(|\boldsymbol{k}| + r + 4)$$

with $w(u, v) = 2^{\alpha_{u+1}+\alpha_{u+2}+\cdots+\alpha_{u+v}}(2^{\alpha_{u+v+1}} - 2)$.

3. A special case of vectorized version

We need to pay a special attention to the integral (2.1) when $\boldsymbol{k} = (p, q)$ and $\mu_1 = 1$, $\mu_2 = -1$. This is equivalent to carry out the shuffle product beginning with the integral

$$\frac{1}{p!q!r!} \iint_{R_1\times R_2} \left(\log\frac{1-t_1}{1-t_2} + \log\frac{1-u_1}{1-u_2}\right)^p \left(-\log\frac{1-t_1}{1-t_2} + \log\frac{1-u_1}{1-u_2}\right)^q$$
$$\times \left(\log\frac{t_2}{t_1} + \log\frac{u_2}{u_1}\right)^r \frac{dt_1dt_2}{(1-t_1)t_2}\frac{du_1du_2}{(1-u_1)u_2}.$$

The value of such integral is

$$\sum_{a+b=p}\sum_{c+d=q} (-1)^c \binom{a+c}{a}\binom{b+d}{b}\sum_{\ell=0}^{r} \zeta(a+c+r-\ell+2)\zeta(b+d+\ell+2)$$

under the same argument mentioned in (2.2). However, we need the following identity to cope with this special case.

Proposition 3.1. *For a pair of nonnegative integers p, q with q even, we have*

$$\sum_{a+b=p}\sum_{c+d=q} (-1)^c \binom{a+c}{a}\binom{b+d}{b} = \binom{p+q+1}{p}. \tag{3.1}$$

Proof. We interpret the sum of products of binomial coefficient of (3.1) as the coefficient of x^q of the rational function

$$\sum_{a+b=p} \frac{1}{(1+x)^{a+1}(1-x)^{b+1}} \tag{3.2}$$

when it was expanded into power series at $x = 0$. Note that the rational function (3.2) is equal to

$$\frac{1}{2x}\left[\frac{1}{(1-x)^{p+1}} - \frac{1}{(1+x)^{p+1}}\right],$$

which has the coefficient of x^q as

$$\frac{1}{2}\left[\binom{p+q+1}{p} - (-1)^{q+1}\binom{p+q+1}{p}\right] = \binom{p+q+1}{p}. \qquad \square$$

Therefore, when q is even, the resulted shuffle relation is given as

$$\sum_{a+b+c=p} 2^{b+1} \sum_{\substack{g+h=q\\ g:\text{even}}} \binom{a+g}{a}\binom{c+h}{c} \sum_{m+n+\ell=r} 2^n \times \sum_{\substack{|\boldsymbol{\alpha}|=a+g+m+1\\ |\boldsymbol{\beta}|=b+n+1\\ |\boldsymbol{\gamma}|=c+h+\ell+1}} \zeta(\alpha_0,\alpha_1,\ldots,\alpha_{a+g},\beta_0,\beta_1,\ldots,\beta_b+\gamma_0,\gamma_1,\ldots,\gamma_{c+h}+1)$$
$$= \frac{1}{2}\binom{p+q+1}{p}\zeta(p+q+r+4).$$

With some refinements in notations, the following identity is obtained.

Theorem 3.2. *For a pair of nonnegative integers p, q with q is even, we have*

$$\sum_{\substack{a+b+c=p\\ g+h=q\\ g:\text{even}}} \binom{a+g}{a}\binom{c+h}{c} \sum_{|\boldsymbol{\alpha}|=p+q+r+3} w(a+g,b)\zeta(\alpha_0,\alpha_1,\ldots,\alpha_{a+g},\ldots,\alpha_{p+q+1}+1)$$
$$= \frac{1}{2}\binom{p+q+1}{p}\zeta(p+q+r+4),$$

with $w(u,v) = 2^{\alpha_{u+1}+\alpha_{u+2}+\cdots+\alpha_{u+v}}(2^{\alpha_{u+v+1}}-2)$.

For the case when q is odd, we begin with the integral with a parameter

$$\frac{1}{p!q!r!}\iint_{R_1\times R_2}\left(\log\frac{1-t_1}{1-t_2}+\log\frac{1-u_1}{1-u_2}\right)^p\left(\mu\log\frac{1-t_1}{1-t_2}+\log\frac{1-u_1}{1-u_2}\right)^q \times\left(\log\frac{t_2}{t_1}+\log\frac{u_2}{u_1}\right)^r\frac{dt_1dt_2}{(1-t_1)t_2}\frac{du_1du_2}{(1-u_1)u_2}. \tag{3.3}$$

Again, under the same argument mentioned in (2.2) as well as the shuffle product process mentioned in [8, pp. 1190–1193], (3.3) is equal to

$$\sum_{a+b=p}\sum_{c+d=q}\mu^c\sum_{m+n=r}\binom{a+c}{a}\binom{b+d}{b}\zeta(a+c+m+2)\zeta(b+d+m+2),$$

and the resulted shuffle relation is given by

$$\begin{aligned}\sum_{a+b=p}\sum_{c+d=q}\mu^c\binom{a+c}{a}\binom{b+d}{b}(r+1)\zeta(p+q+r+4)\\ = \sum_{a+b+c=p}2^b\sum_{g+h+k=q}\sum_{m+n+\ell=r}2^n\binom{a+g}{a}\binom{b+h}{b}\binom{c+k}{c}\\ \times\sum_{\substack{|\boldsymbol{\alpha}|=a+g+m+1\\ |\boldsymbol{\beta}|=b+h+n+1\\ |\boldsymbol{\gamma}|=c+k+\ell+1}}\zeta(\alpha_0,\alpha_1,\ldots,\alpha_{a+g},\beta_0,\beta_1,\ldots,\beta_{b+h}+\gamma_0,\gamma_1,\ldots,\gamma_{c+k}+1)\\ \times\left[(\mu+1)^h(\mu^g+\mu^k+\mu^{g+k}+1)\right].\end{aligned} \tag{3.4}$$

The following basic identity is necessary to our exploration.

Proposition 3.3. *For a pair of nonnegative integers p, q with q odd, we have*

$$\sum_{a+b=p}\sum_{c+d=q}(c+1)(-1)^c\binom{a+c}{a}\binom{b+d}{b} = -\frac{1}{2}(p+1)\binom{p+q+1}{p+1}. \tag{3.5}$$

Proof. The sum involving the binomial coefficients on the left hand side of (3.5)

$$\sum_{a+b=p}\sum_{c+d=q}(c+1)(-1)^c\binom{a+c}{a}\binom{b+d}{b} \tag{3.6}$$

could be obtained by multiplying the double sum

$$\sum_{a+b=p}\sum_{c+d=q}\mu^c\binom{a+c}{a}\binom{b+d}{b} \tag{3.7}$$

by μ; differentiating with respect to μ and then setting $\mu = -1$. However, the double sum (3.7) is the coefficient of x^q of the Taylor expansion at $x = 0$ of the rational function

$$\sum_{a+b=p}\frac{1}{(1-\mu x)^{a+1}(1-x)^{b+1}}, \tag{3.8}$$

which is equal to the following rational function

$$\sum_{a+b=p}\left[\frac{1}{(1+x)^{a+1}(1-x)^{b+1}} - \frac{(a+1)x}{(1+x)^{a+2}(1-x)^{b+1}}\right] \tag{3.9}$$

after executing the same procedure as shown in the derivation of (3.6). Since the coefficient of x^q of the rational function (3.9) is given by

$$-\frac{1}{2}(p+1)\binom{p+q+1}{p+1},$$

our assertion is done. □

In light of Proposition 3.3, the following identity is obtained.

Theorem 3.4. *For a pair of nonnegative integers p, q with q odd, we have*

$$\begin{aligned}
&q\sum_{a+b+c=p}\sum_{\substack{g+h=q\\ g:\text{even}}}\binom{a+g}{a}\binom{c+h}{c}\\
&\quad\times\sum_{|\boldsymbol{\alpha}|=p+q+r+3} w(a+g,b)\zeta(\alpha_0,\alpha_1,\ldots,\alpha_{a+g},\ldots,\alpha_{p+q},\alpha_{p+q+1}+1)\\
&+\sum_{a+b+c=p}\sum_{g+h=q} g(-1)^g\binom{a+g}{a}\binom{c+h}{c}
\end{aligned}$$

$$\times \sum_{|\boldsymbol{\alpha}|=p+q+r+3} w(a+g,b)\zeta(\alpha_0,\alpha_1,\dots,\alpha_{a+g},\dots,\alpha_{p+q},\alpha_{p+q+1}+1)$$
$$+ \sum_{a+b+c=p}\sum_{\substack{g+h=q-1\\ g:\text{even}}} \binom{a+g}{a}\binom{b+1}{b}\binom{c+h}{c}$$
$$\times \sum_{|\boldsymbol{\alpha}|=p+q+r+3} w(a+g,b+1)\zeta(\alpha_0,\alpha_1,\dots,\alpha_{a+g},\dots,\alpha_{p+q},\alpha_{p+q+1}+1)$$
$$= \frac{1}{2}\binom{p+q+1}{p}(p+1)(r+1)\zeta(p+q+r+4),$$

with $w(u,v)=2^{\alpha_{u+1}+\alpha_{u+2}+\cdots+\alpha_{u+v}}(2^{\alpha_{u+v+1}}-2)$.

4. Further generalizations

Let $\boldsymbol{k}=(k_1,k_2,\dots,k_m)$ and $\boldsymbol{r}=(r_1,r_2,\dots,r_n)$ be m-tuple and n-tuple of nonnegative integers, respectively. We shall give the evaluation of the triple product

$$\binom{|\boldsymbol{j}|+|\boldsymbol{r}-\boldsymbol{\ell}|}{|\boldsymbol{j}|}\binom{|\boldsymbol{k}-\boldsymbol{j}|+|\boldsymbol{\ell}|}{|\boldsymbol{\ell}|}\binom{|\boldsymbol{k}|+|\boldsymbol{r}|+4}{|\boldsymbol{j}|+|\boldsymbol{r}-\boldsymbol{\ell}|+2}$$

in the following, where

$$\boldsymbol{j}=(j_1,j_2,\dots,j_m),\qquad 0\le j_i\le k_i,\qquad i=1,2,\dots,m$$

and

$$\boldsymbol{\ell}=(\ell_1,\ell_2,\dots,\ell_n),\qquad 0\le \ell_g\le r_g,\qquad g=1,2,\dots,n.$$

We begin with the integral

$$\frac{1}{\boldsymbol{k}!\boldsymbol{r}!}\iint_{R_1\times R_2}\prod_{i=1}^{m}\left(\mu_i\log\frac{1-t_1}{1-t_2}+\log\frac{1-u_1}{1-u_2}\right)^{k_i}\prod_{g=1}^{n}\left(\log\frac{t_2}{t_1}+\lambda_g\log\frac{u_2}{u_1}\right)^{r_g} \times\frac{dt_1dt_2}{(1-t_1)t_2}\frac{du_1du_2}{(1-u_1)u_2}, \tag{4.1}$$

which has the value

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}}\sum_{\boldsymbol{\gamma}+\boldsymbol{\delta}=\boldsymbol{r}}\boldsymbol{\mu}^{\boldsymbol{\alpha}}\boldsymbol{\lambda}^{\boldsymbol{\delta}}M(\boldsymbol{\alpha})M(\boldsymbol{\gamma})M(\boldsymbol{\beta})M(\boldsymbol{\delta})\zeta(|\boldsymbol{\alpha}|+|\boldsymbol{\gamma}|+2)\zeta(|\boldsymbol{\beta}|+|\boldsymbol{\delta}|+2) \tag{4.2}$$

after the binomial expansions based on the similar argument given in (2.2). However, we need some particular notations in order to develop the generating function of the number of multiple zeta values produced from (4.2).

Given nonnegative integer m, and two vectors $\boldsymbol{u}=(u_1,u_2,\dots,u_n)$ and $\boldsymbol{v}=(v_1,v_2,\dots,v_n)$ with nonnegative integer components, we denote $M(\boldsymbol{u},m)$ and $M(\boldsymbol{u},\boldsymbol{v})$ by

$$\binom{u_1+u_2+\cdots+u_n+m}{u_1,u_2,\dots,u_n,m}=\frac{(u_1+u_2+\cdots+u_n+m)!}{u_1!u_2!\cdots u_n!m!}$$

and
$$\binom{|\boldsymbol{u}|+|\boldsymbol{v}|}{u_1,u_2,\ldots,u_n,v_1,v_2,\ldots,v_n} = \frac{(|\boldsymbol{u}|+|\boldsymbol{v}|)!}{u_1!u_2!\cdots u_n!v_1!v_2!\cdots v_n!},$$
respectively.

Since the number of multiple zeta values regarding to $\zeta(|\boldsymbol{\alpha}|+|\boldsymbol{\gamma}|+2)$ in (4.2) is $\binom{|\boldsymbol{\alpha}|+|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}$ whereas that regarding to $\zeta(|\boldsymbol{\beta}|+|\boldsymbol{\delta}|+2)$ in (4.2) is $\binom{|\boldsymbol{\beta}|+|\boldsymbol{\delta}|}{|\boldsymbol{\delta}|}$ due to the applications of the sum formula (1.2) in (4.2), we conclude that the generating function for the number of multiple zeta values produced from the shuffle product process is

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}}\sum_{\boldsymbol{\gamma}+\boldsymbol{\delta}=\boldsymbol{r}} \boldsymbol{\mu}^{\boldsymbol{\alpha}}\boldsymbol{\lambda}^{\boldsymbol{\delta}} M(\boldsymbol{\alpha},\boldsymbol{\gamma})M(\boldsymbol{\beta},\boldsymbol{\delta})\binom{|\boldsymbol{k}|+|\boldsymbol{r}|+4}{|\boldsymbol{\alpha}|+|\boldsymbol{\gamma}|+2} \tag{4.3}$$

with the help of the trivial identity

$$M(\boldsymbol{u},\boldsymbol{v}) = \binom{|\boldsymbol{u}|+|\boldsymbol{v}|}{|\boldsymbol{v}|}M(\boldsymbol{u})M(\boldsymbol{v}).$$

We introduce two useful propositions before entering the shuffle process.

Proposition 4.1. *For nonnegative integers m,n,k and μ, let*

$$P(m,n,k;\mu) = \sum_{a+b=k}(\mu+1)^b\binom{m+a}{m}\binom{n+b}{n}. \tag{4.4}$$

Then for $0\le j\le k$, the coefficient of μ^j of $P(m,n,k;\mu)$ is

$$\binom{n+j}{j}\binom{m+n+k+1}{k-j}.$$

That is,

$$P(m,n,k;\mu) = \sum_{j=0}^{k}\binom{n+j}{j}\binom{m+n+k+1}{k-j}\mu^j.$$

Proof. As
$$\frac{1}{(1-x)^{m+1}} = \sum_{a=0}^{\infty}\binom{m+a}{m}x^a$$
and
$$\frac{1}{[1-(\mu+1)x]^{n+1}} = \sum_{b=0}^{\infty}(\mu+1)^b\binom{n+b}{n}x^b$$
so that $P(m,n,k;\mu)$ is just the coefficient of x^k of the product
$$\frac{1}{(1-x)^{m+1}}\frac{1}{[1-(\mu+1)x]^{n+1}}.$$

The coefficient of μ^j of the above product is

$$\begin{aligned}&\frac{1}{j!}\left(\frac{\partial}{\partial\mu}\right)^j\left[\frac{1}{(1-x)^{m+1}}\frac{1}{[1-(\mu+1)x]^{n+1}}\right]\Bigg|_{\mu=0}\\ =&\binom{n+j}{j}\frac{x^j}{(1-x)^{m+n+j+2}}.\end{aligned}$$

Note that the coefficient of μ^j in $P(m,n,k;\mu)$ is equal to the coefficient of x^k in

$$\binom{n+j}{j}\frac{x^j}{(1-x)^{m+n+j+2}}$$

which is

$$\binom{n+j}{j}\binom{m+n+k+1}{k-j}.$$

□

For nonnegative integers m,n,k and μ, let

$$\begin{aligned}Q(m,n,k;\mu)&=\sum_{a+b=k}\mu^a(\mu+1)^b\binom{m+a}{m}\binom{n+b}{n}\\ &=\mu^k\sum_{a+b=k}(\mu^{-1}+1)^b\binom{m+a}{m}\binom{n+b}{n}.\end{aligned}\tag{4.5}$$

Corollary 4.2. *Notation as above, then the coefficient of μ^j of $Q(m,n,k;\mu)$ for $0\le j\le k$ is*

$$\binom{n+k-j}{k-j}\binom{m+n+k+1}{j}.$$

The vectorized version of the above conclusion is given as follows.

Proposition 4.3. *Let m be a nonnegative integer and $\boldsymbol{k}=(k_1,k_2,\dots,k_n)$, $\boldsymbol{j}=(j_1,j_2,\dots,j_n)$ with $0\le j_i\le k_i$, $i=1,2,\dots,n$ be n-tuples of nonnegative integers. Then the coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}$ of the polynomial*

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}}(\boldsymbol{\mu}+1)^{\boldsymbol{\alpha}}M(\boldsymbol{\alpha})M(\boldsymbol{\beta},m)\tag{4.6}$$

is

$$\binom{m+|\boldsymbol{k}|+1}{|\boldsymbol{k}-\boldsymbol{j}|}M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j}).$$

Proof. Note that

$$M(\boldsymbol{\alpha})=\binom{|\boldsymbol{\alpha}|}{\alpha_1}M\left((\alpha_2,\dots,\alpha_n)\right)$$

and

$$M(\boldsymbol{\beta},m)=\binom{|\boldsymbol{\beta}|+m}{\beta_1}M\left((\beta_2,\dots,\beta_n),m\right)$$

and the coefficient of $\mu_1^{j_1}$ of the polynomial

$$\sum_{\alpha_1+\beta_1=k_1} \binom{|\boldsymbol{\alpha}|}{\alpha_1}\binom{|\boldsymbol{\beta}|+m}{\beta_1}(\mu_1+1)^{\alpha_1}$$

is

$$\binom{\alpha_2+\cdots+\alpha_n+j_1}{j_1}\binom{m+|\boldsymbol{k}|+1}{k_1-j_1}.$$

Therefore the coefficient of $\mu_1^{j_1}$ in the polynomial (4.6) is

$$\binom{m+|\boldsymbol{k}|+1}{k_1-j_1}\sum(\mu_2+1)^{\alpha_2}\cdots(\mu_n+1)^{\alpha_n}M\left((\alpha_2,\ldots,\alpha_n),j_1\right)M\left((\beta_2,\ldots,\beta_n),m\right),$$

where the summation is taking over $\alpha_i+\beta_i$ for $i=2,3,\ldots,n$. By repeating same process $(n-1)$ times, we obtain the coefficient of μ^j of the polynomial (4.6) is

$$\binom{m+|\boldsymbol{k}|+1}{k_1-j_1,k_2-j_2,\ldots,k_n-j_n,m+|\boldsymbol{j}|+1}M(\boldsymbol{j})$$

or

$$M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j})\binom{m+|\boldsymbol{k}|+1}{|\boldsymbol{k}-\boldsymbol{j}|}. \qquad \square$$

Corollary 4.4. *If m and n are two nonnegative integers and $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, $\boldsymbol{k}$ are three vectors with nonnegative integer components, then we have the followings.*

(1) *The coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}$ of the polynomial*

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}}(\boldsymbol{\mu}+1)^{\boldsymbol{\beta}}M(\boldsymbol{\alpha},m)M(\boldsymbol{\beta},n)$$

is

$$\binom{n+|\boldsymbol{j}|}{|\boldsymbol{j}|}\binom{m+n+|\boldsymbol{k}|+1}{|\boldsymbol{k}-\boldsymbol{j}|}M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j}).$$

(2) *The coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}$ of the polynomial*

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}}\boldsymbol{\mu}^{\boldsymbol{\alpha}}(\boldsymbol{\mu}+1)^{\boldsymbol{\beta}}M(\boldsymbol{\alpha},m)M(\boldsymbol{\beta},n)$$

is

$$\binom{n+|\boldsymbol{k}-\boldsymbol{j}|}{|\boldsymbol{k}-\boldsymbol{j}|}\binom{m+n+|\boldsymbol{k}|+1}{|\boldsymbol{j}|}M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j}).$$

Now, let's begin the shuffle process of the integration (4.1) over the following six simplices:

$$D_1:\ 0<t_1<t_2<u_1<u_2<1,\quad D_2:\ 0<u_1<u_2<t_1<t_2<1,$$
$$D_3:\ 0<t_1<u_1<t_2<u_2<1,\quad D_4:\ 0<t_1<u_1<u_2<t_2<1,$$
$$D_5:\ 0<u_1<t_1<u_2<t_2<1,\quad D_6:\ 0<u_1<t_1<t_2<u_2<1.$$

On the first simplex $D_1:\ 0 < t_1 < t_2 < u_1 < u_2 < 1$, replace the factors

$$\left(\mu_i \log\frac{1-t_1}{1-t_2} + \log\frac{1-u_1}{1-u_2}\right)^{k_i}$$

and

$$\left(\log\frac{t_2}{t_1} + \lambda_g \log\frac{u_2}{u_1}\right)^{r_g}$$

by

$$\sum_{\alpha_i+\beta_i=k_i} \frac{k_i!}{\alpha_i!\beta_i!}\left(\mu_i \log\frac{1-t_1}{1-t_2}\right)^{\alpha_i}\left(\log\frac{1-u_1}{1-u_2}\right)^{\beta_i},\ i=1,2,\ldots,m$$

and

$$\sum_{\rho_j+\upsilon_j=r_j} \frac{r_j!}{\rho_j!\upsilon_j!}\left(\log\frac{t_2}{t_1}\right)^{\rho_i}\left(\lambda_g \log\frac{u_2}{u_1}\right)^{\upsilon_j},\ g=1,2,\ldots,n,$$

respectively, then the generating function for the number of multiple zeta values is

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}=\boldsymbol{k}}\ \sum_{\boldsymbol{\rho}+\boldsymbol{\upsilon}=\boldsymbol{r}} \boldsymbol{\mu}^{\boldsymbol{\alpha}}\boldsymbol{\lambda}^{\boldsymbol{\upsilon}} M(\boldsymbol{\alpha},\boldsymbol{\rho})M(\boldsymbol{\beta},\boldsymbol{\upsilon}), \tag{4.7}$$

and the coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}\boldsymbol{\lambda}^{\boldsymbol{\ell}}$ is

$$M(\boldsymbol{j},\boldsymbol{\gamma}-\boldsymbol{\ell})M(\boldsymbol{k}-\boldsymbol{j},\boldsymbol{\ell}),$$

which is equal to

$$M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j})M(\boldsymbol{\ell})M(\boldsymbol{r}-\boldsymbol{\ell})\binom{|\boldsymbol{j}|+|\boldsymbol{r}-\boldsymbol{\ell}|}{|\boldsymbol{r}-\boldsymbol{\ell}|}\binom{|\boldsymbol{k}-\boldsymbol{j}|+|\boldsymbol{\ell}|}{|\boldsymbol{\ell}|}.$$

Since the integration (4.1) over D_2 produces the same generating function of the integration over D_1, we conclude that the coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}\boldsymbol{\lambda}^{\boldsymbol{\ell}}$ of (4.7) over D_1 and D_2 is given as

$$2M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j})M(\boldsymbol{\ell})M(\boldsymbol{r}-\boldsymbol{\ell})\binom{|\boldsymbol{j}|+|\boldsymbol{r}-\boldsymbol{\ell}|}{|\boldsymbol{r}-\boldsymbol{\ell}|}\binom{|\boldsymbol{k}-\boldsymbol{j}|+|\boldsymbol{\ell}|}{|\boldsymbol{\ell}|}. \tag{4.8}$$

Similarly, the integration over D_5 also produces the same generating function of the integration over D_3, so we only consider the partial generating function over D_3 in what follows.

On the simplex $D_3:\ 0 < t_1 < u_1 < t_2 < u_2 < 1$, replace the factors

$$\left(\mu_i \log\frac{1-t_1}{1-t_2} + \log\frac{1-u_1}{1-u_2}\right)^{k_i}$$

and

$$\left(\log\frac{t_2}{t_1} + \lambda_g \log\frac{u_2}{u_1}\right)^{r_g}$$

by

$$\sum_{\alpha_i+\beta_i+\gamma_i=k_i}\frac{k_i!}{\alpha_i!\beta_i!\gamma_i!}\left(\mu_i\log\frac{1-t_1}{1-u_1}\right)^{\alpha_i}\left((\mu_i+1)\log\frac{1-u_1}{1-t_2}\right)^{\beta_i}\left(\log\frac{1-t_2}{1-u_2}\right)^{\gamma_i}$$

for $i=1,2,\ldots,m$ and

$$\sum_{\rho_j+\upsilon_j+\omega_j=r_j}\frac{r_j!}{\rho_j!\upsilon_j!\omega_j!}\left(\log\frac{u_1}{t_1}\right)^{\rho_j}\left((\lambda_g+1)\log\frac{t_2}{u_1}\right)^{\upsilon_j}\left(\lambda_g\log\frac{u_2}{t_2}\right)^{\omega_j}$$

for $g=1,2,\ldots,n$, respectively. Then the generating function for the number of multiple zeta values is

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}=\boldsymbol{k}}\boldsymbol{\mu}^{\boldsymbol{\alpha}}(\boldsymbol{\mu}+1)^{\boldsymbol{\beta}}\sum_{\boldsymbol{\rho}+\boldsymbol{\upsilon}+\boldsymbol{\omega}=\boldsymbol{r}}(\boldsymbol{\lambda}+1)^{\boldsymbol{\upsilon}}\boldsymbol{\lambda}^{\boldsymbol{\omega}}M(\boldsymbol{\alpha},\boldsymbol{\rho})M(\boldsymbol{\beta},\boldsymbol{\upsilon})M(\boldsymbol{\gamma},\boldsymbol{\omega}), \tag{4.9}$$

which is equal to

$$\begin{aligned}\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}=\boldsymbol{k}}\boldsymbol{\mu}^{\boldsymbol{\alpha}}(\boldsymbol{\mu}+1)^{\boldsymbol{\beta}}\sum_{\boldsymbol{\rho}+\boldsymbol{\upsilon}+\boldsymbol{\omega}=\boldsymbol{r}}&(\boldsymbol{\lambda}+1)^{\boldsymbol{\upsilon}}\boldsymbol{\lambda}^{\boldsymbol{\omega}}M(\boldsymbol{\rho},|\boldsymbol{\alpha}|)M(\boldsymbol{\upsilon},|\boldsymbol{\beta}|)M(\boldsymbol{\omega},|\boldsymbol{\gamma}|)\\ &\times M(\boldsymbol{\alpha})M(\boldsymbol{\beta})M(\boldsymbol{\gamma}).\end{aligned} \tag{4.10}$$

For the coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}\boldsymbol{\lambda}^{\boldsymbol{\ell}}$ of the polynomial (4.9), we consider the coefficient of $\boldsymbol{\lambda}^{\boldsymbol{\ell}-\boldsymbol{\omega}}$ of the polynomial

$$\sum_{\boldsymbol{\rho}+\boldsymbol{\upsilon}+\boldsymbol{\omega}=\boldsymbol{r}}(\boldsymbol{\lambda}+1)^{\boldsymbol{\upsilon}}M(\boldsymbol{\rho},|\boldsymbol{\alpha}|)M(\boldsymbol{\upsilon},|\boldsymbol{\beta}|) \tag{4.11}$$

first. Merge the dummy variables $\boldsymbol{r}$ and $\boldsymbol{\omega}$ via Corollary 4.4 leads to the coefficient of $\boldsymbol{\lambda}^{\boldsymbol{\ell}-\boldsymbol{\omega}}$ of (4.11) in what follows

$$\binom{|\boldsymbol{\beta}|+|\boldsymbol{\ell}-\boldsymbol{\omega}|}{|\boldsymbol{\ell}-\boldsymbol{\omega}|}\binom{|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|+|\boldsymbol{r}-\boldsymbol{\omega}|+1}{|\boldsymbol{r}-\boldsymbol{\ell}|}M(\boldsymbol{\ell}-\boldsymbol{\omega})M(\boldsymbol{r}-\boldsymbol{\ell}), \tag{4.12}$$

which is the coefficient of $\boldsymbol{\lambda}^{\boldsymbol{\ell}}$ of the polynomial

$$\sum_{\boldsymbol{\rho}+\boldsymbol{\upsilon}+\boldsymbol{\omega}=\boldsymbol{r}}(\boldsymbol{\lambda}+1)^{\boldsymbol{\upsilon}}\boldsymbol{\lambda}^{\boldsymbol{\omega}}M(\boldsymbol{\rho},|\boldsymbol{\alpha}|)M(\boldsymbol{\upsilon},|\boldsymbol{\beta}|). \tag{4.13}$$

Therefore, the coefficient of $\boldsymbol{\lambda}^{\boldsymbol{\ell}}$ of the polynomial

$$\sum_{\boldsymbol{\rho}+\boldsymbol{\upsilon}+\boldsymbol{\omega}=\boldsymbol{r}}(\boldsymbol{\lambda}+1)^{\boldsymbol{\upsilon}}\boldsymbol{\lambda}^{\boldsymbol{\omega}}M(\boldsymbol{\rho},|\boldsymbol{\alpha}|)M(\boldsymbol{\upsilon},|\boldsymbol{\beta}|)M(\boldsymbol{\omega},|\boldsymbol{\gamma}|) \tag{4.14}$$

is given by

(4.15)
$$\sum_{m+n=|\boldsymbol{\ell}|}\binom{m+|\boldsymbol{\beta}|}{m}\binom{n+|\boldsymbol{r}|}{n}\binom{|\boldsymbol{\alpha}|+|\boldsymbol{\beta}|+|\boldsymbol{r}-\boldsymbol{\ell}|+m+1}{|\boldsymbol{r}-\boldsymbol{\ell}|}M(\boldsymbol{\ell}-\boldsymbol{\omega})M(\boldsymbol{\omega})M(\boldsymbol{r}-\boldsymbol{\ell})$$

if we set $m = |\boldsymbol{\ell} - \boldsymbol{\omega}|$ and $n = |\boldsymbol{\omega}|$.

On the other hand, the coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}$ of the polynomial

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}=\boldsymbol{k}} \boldsymbol{\mu}^{\boldsymbol{\alpha}}(\boldsymbol{\mu}+1)^{\boldsymbol{\beta}} M(\boldsymbol{\beta}, m) M(\boldsymbol{\alpha}) \tag{4.16}$$

is given by

$$\binom{m + |\boldsymbol{k}-\boldsymbol{\gamma}-\boldsymbol{j}|}{|\boldsymbol{k}-\boldsymbol{\gamma}-\boldsymbol{j}|}\binom{|\boldsymbol{k}-\boldsymbol{\gamma}|+m+1}{|\boldsymbol{j}|} M(\boldsymbol{j}) M(\boldsymbol{k}-\boldsymbol{\gamma}-\boldsymbol{j}) \tag{4.17}$$

in light of Corollary 4.4 after merging two dummy variables $\boldsymbol{k}$ and $\boldsymbol{\gamma}$. Consequently, the coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}\boldsymbol{\lambda}^{\boldsymbol{\ell}}$ of the polynomial (4.9) is given by

$$\begin{aligned} &M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j})M(\boldsymbol{\ell})M(\boldsymbol{r}-\boldsymbol{\ell}) \\ &\quad\times \sum_{a+b=|\boldsymbol{k}-\boldsymbol{j}|} \sum_{m+n=|\boldsymbol{\ell}|} \binom{a+m}{a}\binom{b+n}{b}\binom{a+m+|\boldsymbol{j}|+|\boldsymbol{r}-\boldsymbol{\ell}|+1}{|\boldsymbol{r}-\boldsymbol{\ell}|, |\boldsymbol{j}|, a+m+1} \end{aligned} \tag{4.18}$$

if we set $a = |\boldsymbol{k}-\boldsymbol{\gamma}-\boldsymbol{j}|$ and $b = |\boldsymbol{\gamma}|$.

In the same manner, we obtain the generating functions over $D_4 :\ 0 < t_1 < u_1 < u_2 < t_2 < 1$ and $D_6 :\ 0 < u_1 < t_1 < t_2 < u_2 < 1$ as

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}=\boldsymbol{k}} \boldsymbol{\mu}^{\boldsymbol{\alpha}+\boldsymbol{\gamma}}(\boldsymbol{\mu}+1)^{\boldsymbol{\beta}} \sum_{\boldsymbol{\rho}+\boldsymbol{v}+\boldsymbol{\omega}=\boldsymbol{r}} (\boldsymbol{\lambda}+1)^{\boldsymbol{v}} M(\boldsymbol{\alpha},\boldsymbol{\rho}) M(\boldsymbol{\beta},\boldsymbol{v}) M(\boldsymbol{\gamma},\boldsymbol{\omega}), \tag{4.19}$$

and

$$\sum_{\boldsymbol{\alpha}+\boldsymbol{\beta}+\boldsymbol{\gamma}=\boldsymbol{k}} (\boldsymbol{\mu}+1)^{\boldsymbol{\beta}} \sum_{\boldsymbol{\rho}+\boldsymbol{v}+\boldsymbol{\omega}=\boldsymbol{r}} (\boldsymbol{\lambda}+1)^{\boldsymbol{v}} \boldsymbol{\lambda}^{\boldsymbol{v}+\boldsymbol{\omega}} M(\boldsymbol{\alpha},\boldsymbol{\rho}) M(\boldsymbol{\beta},\boldsymbol{v}) M(\boldsymbol{\gamma},\boldsymbol{\omega}), \tag{4.20}$$

respectively. With the help of Corollary 4.4, the coefficients of $\boldsymbol{\mu}^{\boldsymbol{j}}\boldsymbol{\lambda}^{\boldsymbol{\ell}}$ of (4.19) and (4.20) are given as

$$M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j})M(\boldsymbol{\ell})M(\boldsymbol{r}-\boldsymbol{\ell})\binom{|\boldsymbol{k}|+|\boldsymbol{r}|+2}{|\boldsymbol{j}|}\binom{|\boldsymbol{k}-\boldsymbol{j}|+|\boldsymbol{\ell}|}{|\boldsymbol{\ell}|}\binom{|\boldsymbol{r}|+|\boldsymbol{k}-\boldsymbol{j}|+2}{|\boldsymbol{r}-\boldsymbol{\ell}|} \tag{4.21}$$

and

$$M(\boldsymbol{j})M(\boldsymbol{k}-\boldsymbol{j})M(\boldsymbol{\ell})M(\boldsymbol{r}-\boldsymbol{\ell})\binom{|\boldsymbol{k}|+|\boldsymbol{r}|+2}{|\boldsymbol{k}-\boldsymbol{j}|}\binom{|\boldsymbol{j}|+|\boldsymbol{r}-\boldsymbol{\ell}|}{|\boldsymbol{r}-\boldsymbol{\ell}|}\binom{|\boldsymbol{r}|+|\boldsymbol{j}|+2}{|\boldsymbol{\ell}|}, \tag{4.22}$$

respectively. It is evident that $(4.3) = 2\times(4.7) + 2\times(4.9) + (4.19) + (4.20)$. By comparing the coefficient of $\boldsymbol{\mu}^{\boldsymbol{j}}\boldsymbol{\lambda}^{\boldsymbol{\ell}}$ on both sides of the above identity, we conclude the following theorem.

Theorem 4.5. *For nonnegative integers a, b, m and n, and the vectors with nonnegative integer components $\boldsymbol{k} = (k_1, k_2, \ldots, k_m)$, $\boldsymbol{r} = (r_1, r_2, \ldots, r_n)$,*

$$\boldsymbol{j} = (j_1, j_2, \ldots, j_m), \qquad 0 \leq j_i \leq k_i, \qquad i = 1, 2, \ldots, m$$

and

$$\boldsymbol{\ell} = (\ell_1, \ell_2, \ldots, \ell_n), \qquad 0 \leq \ell_g \leq r_g, \qquad g = 1, 2, \ldots, n,$$

we have

$$\begin{aligned}
&\binom{|\boldsymbol{j}| + |\boldsymbol{r} - \boldsymbol{\ell}|}{|\boldsymbol{j}|}\binom{|\boldsymbol{k} - \boldsymbol{j}| + |\boldsymbol{\ell}|}{|\boldsymbol{\ell}|}\left\{\binom{|\boldsymbol{k}| + |\boldsymbol{r}| + 4}{|\boldsymbol{j}| + |\boldsymbol{r} - \boldsymbol{\ell}| + 2} - 2\right\} \\
&= \binom{|\boldsymbol{k}| + |\boldsymbol{r}| + 2}{|\boldsymbol{j}|}\binom{|\boldsymbol{k} - \boldsymbol{j}| + |\boldsymbol{\ell}|}{|\boldsymbol{\ell}|}\binom{|\boldsymbol{r}| + |\boldsymbol{k} - \boldsymbol{j}| + 2}{|\boldsymbol{r} - \boldsymbol{\ell}|} \\
&\quad + \binom{|\boldsymbol{k}| + |\boldsymbol{r}| + 2}{|\boldsymbol{k} - \boldsymbol{j}|}\binom{|\boldsymbol{j}| + |\boldsymbol{r} - \boldsymbol{\ell}|}{|\boldsymbol{r} - \boldsymbol{\ell}|}\binom{|\boldsymbol{r}| + |\boldsymbol{j}| + 2}{|\boldsymbol{\ell}|} \\
&\quad + 2 \sum_{a+b=|\boldsymbol{k}-\boldsymbol{j}|} \sum_{m+n=|\boldsymbol{\ell}|} \binom{a+m}{a}\binom{b+n}{b}\binom{a+m+1+|\boldsymbol{j}|+|\boldsymbol{r}-\boldsymbol{\ell}|}{a+m+1, |\boldsymbol{j}|, |\boldsymbol{r}-\boldsymbol{\ell}|}.
\end{aligned} \tag{4.23}$$

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