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Some alternating double sum formulae of multiple zeta values

MINKING EIE[1], FU-YAO YANG[2] and YAO LIN ONG[3]

[1]Department of Mathematics, National Chung Cheng University, 168 University Rd. Minhsiung, Chiayi 62145, Taiwan

[2]Department of Information Management, Toko University, 51 University Rd. Sec. 2, Pu-Tzu, Chiayi 613, Taiwan

[3]Department of Accounting and Information System, Chang Jung Christian University, Kway-Jen, Tainan 711, Taiwan

E-mails: minking@math.ccu.edu.tw / vipent@mail.toko.edu.tw / ylong@mail.cjcu.edu.tw

Abstract. In this paper, we produce shuffle relations from multiple zeta values of the form $\zeta(\{1\}^{m-1}, n+1)$. Here $\{1\}^k$ is k repetitions of 1, and for a string of positive integers α_1, α_2, $\ldots, \alpha_r$ with $\alpha_r \geq 2$

$$\zeta(\alpha_1, \alpha_2, \ldots, \alpha_r) = \sum_{1 \leq n_1 < n_2 < \ldots < n_r} n_1^{-\alpha_1} n_2^{-\alpha_2} \cdots n_r^{-\alpha_r}.$$

As applications of the sum formula and a newly developed weighted sum formula, we shall prove for even integers $k, r \geq 0$ that

$$\sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{\ell} \sum_{\substack{|\boldsymbol{\alpha}|=j+r-\ell+1 \\ |\boldsymbol{\beta}|=k-j+\ell+2}} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_j + \beta_j, \beta_{j+1}, \ldots, \beta_k, \beta_{k+1} + 1)$$

$$+ \sum_{\substack{0 \leq \ell \leq r \\ \ell:\text{even}}} \sum_{|\boldsymbol{\alpha}|=k+\ell+1} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, r-\ell+3) \;=\; \zeta(k+r+4).$$

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1 Introduction

For a pair of positive integers p and q with $q \geq 2$, the classical Euler sum $S_{p,q}$ is defined as [2, 3, 8, 10]

$$S_{p,q} := \sum_{k=1}^{\infty} \frac{1}{k^q} \sum_{j=1}^{k} \frac{1}{j^p}.$$

The number $p+q$ is the weight of $S_{p,q}$. When $p = 1$, or $(p,q) = (2,4)$, or $(p,q) = (4,2)$, or $p = q$, or $p+q$ is odd, $S_{p,q}$ can be expressed in terms of the special values of Riemann zeta function at positive integers. See [12, 13, 14] for the details of evaluations.

Multiple zeta values are multidimensional version of the Euler sums [1, 6, 9, 13, 14, 15]. For a string of positive integers $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_r)$ with $\alpha_r \geq 2$, the multiple zeta value or r-fold Euler sum $\zeta(\alpha_1, \alpha_2, \ldots, \alpha_r)$ is defined as

$$\zeta(\boldsymbol{\alpha}) = \zeta(\alpha_1, \alpha_2, \ldots, \alpha_r) := \sum_{k_r=1}^{\infty} \frac{1}{k_r^{\alpha_r}} \cdots \sum_{k_2=1}^{k_3-1} \frac{1}{k_2^{\alpha_2}} \sum_{k_1=1}^{k_2-1} \frac{1}{k_1^{\alpha_1}},$$

or equivalently as

$$\sum_{1 \leq n_1 < n_2 < \cdots < n_r} n_1^{-\alpha_1} n_2^{-\alpha_2} \cdots n_r^{-\alpha_r}.$$

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

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

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

There is an integral representation, due to Kontsevich [4, 5, 13], to express multiple zeta values in terms of iterated integrals (or Drinfeld integrals) over simplices of weight-dimension, namely,

$$\zeta(\alpha_1, \alpha_2, \ldots, \alpha_r) = \int_{0<t_1<t_2<\cdots<t_{|\boldsymbol{\alpha}|}<1} \Omega_1 \Omega_2 \cdots \Omega_{|\boldsymbol{\alpha}|},$$

where

$$\Omega_j = dt_j/(1-t_j) \ \text{ if } \ j \in \{1, \alpha_1+1, \alpha_1+\alpha_2+1, \ldots, \alpha_1+\cdots+\alpha_{r-1}+1\}$$

and $\Omega_j = dt_j/t_j$, otherwise. For our convenience, we rewrite the above integral representation as

$$\int_0^1 \Omega_1\Omega_2\cdots\Omega_{|\boldsymbol{\alpha}|}.$$

An elementary consideration yields a depth-dimensional integral representation as

$$\zeta(\alpha_1,\alpha_2,\ldots,\alpha_r) = \frac{1}{(\alpha_1-1)!(\alpha_2-1)!\cdots(\alpha_r-1)!}$$

$$\times\int_{0<t_1<t_2<\cdots<t_r<1} \frac{dt_1}{1-t_1}\left(\log\frac{t_2}{t_1}\right)^{\alpha_1-1}\frac{dt_2}{1-t_2}\left(\log\frac{t_3}{t_2}\right)^{\alpha_2-1}\cdots$$

$$\cdots\frac{dt_r}{1-t_r}\left(\log\frac{1}{t_r}\right)^{\alpha_r-1}.$$

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

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

from which the so-called Drinfeld duality theorem

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

follows easily.

The above Drinfeld integral representation for multiple zeta values also enables us to express the product of two multiple zeta values as a linear combination of multiple zeta values through the shuffle product formula of two multiple zeta values. The shuffle product formula of two multiple zeta values is defined as

$$\int_0^1 \Omega_1\Omega_2\cdots\Omega_m\int_0^1 \Omega_{m+1}\Omega_{m+2}\cdots\Omega_{m+n} = \sum_{\sigma}\int_0^1 \Omega_{\sigma(1)}\Omega_{\sigma(2)}\cdots\Omega_{\sigma(m+n)},$$

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 $1 \leq i < j \leq m$ and $m+1 \leq i < j \leq m+n$.

We restrict our attention to shuffle product formulae obtained from a group of multiple zeta values of the form $\zeta(\{1\}^{m-1}, n+1)$, which can be further expressed as integrals in one variable or double integrals in two variables. The following propositions are main tools for our exploration.

Proposition 1. [7] *For a pair of positive integers m and n, we have*

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

$$= \frac{1}{(m-1)!(n-1)!} \int_{0<t_1<t_2<1} \left(\log \frac{1}{1-t_1}\right)^{m-1} \left(\log \frac{1}{t_2}\right)^{n-1} \frac{dt_1 dt_2}{(1-t_1)t_2}$$

$$= \frac{1}{(m-1)!(n-1)!} \int_{0<t_1<t_2<1} \left(\log \frac{1-t_1}{1-t_2}\right)^{m-1} \left(\log \frac{1}{t_2}\right)^{n-1} \frac{dt_1 dt_2}{(1-t_1)t_2}.$$

Proposition 2. [7] *For an integer $p \geq 0$ and positive integers q, m and n with $m \geq q$, we have*

$$\sum_{|\boldsymbol{\alpha}|=m} \zeta(\{1\}^p, \alpha_1, \alpha_2, \ldots, \alpha_q + n)$$

$$= \frac{1}{p!(q-1)!(m-q)!(n-1)!} \int_{0<t_1<t_2<1} \left(\log \frac{1}{1-t_1}\right)^p \left(\log \frac{1-t_1}{1-t_2}\right)^{q-1}$$

$$\times \left(\log \frac{t_2}{t_1}\right)^{m-q} \left(\log \frac{1}{t_2}\right)^{n-1} \frac{dt_1 dt_2}{(1-t_1)t_2}.$$

In particular, for integers k, $r \geq 0$, one has

$$\sum_{|\boldsymbol{\alpha}|=k+r+1} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k + 1)$$

$$= \frac{1}{k!r!} \int_{0<t_1<t_2<1} \left(\log \frac{1-t_1}{1-t_2}\right)^k \left(\log \frac{t_2}{t_1}\right)^r \frac{dt_1 dt_2}{(1-t_1)t_2}.$$

Proposition 3. [13] *For positive integers $a_1, b_1, a_2, b_2, \ldots, a_r, b_r$, let*

$$\mathbf{p} = \left(\{1\}^{a_1-1}, b_1+1, \{1\}^{a_2-1}, b_2+1, \ldots, \{1\}^{a_r-1}, b_r+1\right)$$

and $\mathbf{p}'$ *be the dual of* $\mathbf{p}$,

$$\mathbf{p}' = \left(\{1\}^{b_r-1}, a_r+1, \ldots, \{1\}^{b_2-1}, a_2+1, \{1\}^{b_1-1}, a_1+1\right).$$

Then for any integer $\ell \geq 0$, *we have*

$$\sum_{|\mathbf{c}|=\ell} \zeta(\mathbf{p}+\mathbf{c}) = \sum_{|\mathbf{d}|=\ell} \zeta(\mathbf{p}'+\mathbf{d}).$$

In this paper, we shall consider integrals of the form

$$\frac{1}{k!r!}\int_{0<t_1<t_2<1}\int_{0<u_1<u_2<1}\left(\log\frac{1-t_1}{1-u_1}\right)^k\left(\log\frac{u_2}{t_1}+\log\frac{u_2}{u_1}\right)^r \times\frac{dt_1dt_2}{(1-t_1)t_2}\frac{du_1du_2}{(1-u_1)u_2}$$

which can be expressed as a finite sum of products of multiple zeta values of the form $\zeta(\{1\}^{m-1}, n+1)$. All possible interlacing of the variables t_1, t_2 and u_1, u_2 then produce 6 simplices. Integrations over each simplex give another expression in terms of 6 sums of multiple zeta values. Our alternating double sum of multiple zeta values is just one among them.

Theorem 4. *For a pair of even integers* $k, r \geq 0$, *we have*

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^\ell \sum_{\substack{|\boldsymbol{\alpha}|=j+r-\ell+1\\ |\boldsymbol{\beta}|=k-j+\ell+1}} \zeta(\alpha_0,\alpha_1,\ldots,\alpha_j+\beta_j,\beta_{j+1},\ldots,\beta_k,2) = \sum_{|\boldsymbol{\alpha}|=k+r+2}\zeta(\alpha_0,\alpha_1,\ldots,\alpha_k,2).$$

Theorem 5. *For a pair of even integers* $k, r \geq 0$, *we have*

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^\ell \sum_{\substack{|\boldsymbol{\alpha}|=j+r-\ell+1\\ |\boldsymbol{\beta}|=k-j+\ell+2}} \zeta(\alpha_0,\alpha_1,\ldots,\alpha_j+\beta_j,\beta_{j+1},\ldots,\beta_k,\beta_{k+1}+1) + \sum_{\substack{0\leq\ell\leq r\\ \ell:\mathit{even}}}\sum_{|\boldsymbol{\alpha}|=k+\ell+1}\zeta(\alpha_0,\alpha_1,\ldots,\alpha_k,r-\ell+3) = \zeta(k+r+4).$$

Some extensions of these theorems would be discussed in section 4.

2 Shuffle relations and the sum formula

In 1997, A. Granville proved the sum formula

$$\sum_{|\boldsymbol{\alpha}|=m} \zeta(\alpha_1, \alpha_2, \ldots, \alpha_r + 1) = \zeta(m+1)$$

which was originally conjectured independently by C. Moen and M. Schmidt around 1990 [11, 12, 13]. Also he mentioned that it was proved independently by Zagier in one of his unpublished papers. Here we show that the sum formula is equivalent to the evaluations of multiple zeta values of the form $\zeta(\{1\}^{m-1}, n+1)$.

Proposition 6. *For a pair of integers $k, r \geq 0$, we have*

$$\begin{aligned}
&\left\{1 + (-1)^{k+r}\right\} \sum_{|\boldsymbol{\alpha}|=k+r+3} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1} + 1) \\
&\quad + \left\{(-1)^k + (-1)^r\right\} \zeta(\{1\}^{k+1}, r+3) \\
&= \sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{j+\ell} \zeta(\{1\}^j, r-\ell+2) \zeta(\{1\}^{k-j}, \ell+2).
\end{aligned}$$

In particular, when $k + r$ is even

$$\begin{aligned}
&\sum_{|\boldsymbol{\alpha}|=k+r+3} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1} + 1) + (-1)^k \zeta(\{1\}^{k+1}, r+3) \\
&= \frac{1}{2} \sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{j+\ell} \zeta(\{1\}^j, r-\ell+2) \zeta(\{1\}^{k-j}, \ell+2).
\end{aligned}$$

Proof. We begin with the integral

$$\frac{1}{k!r!} \int_{0<t_1<t_2<1} \int_{0<u_1<u_2<1} \left(\log \frac{1-t_1}{1-u_1}\right)^k \left(\log \frac{u_2}{t_2}\right)^r \frac{dt_1 dt_2}{(1-t_1)t_2} \frac{du_1 du_2}{(1-u_1)u_2}.$$

Rewriting the integrand of the above integral as

$$\sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{j+\ell} \frac{k!r!}{j!(k-j)!\ell!(r-\ell)!}$$

$$\times \left(\log \frac{1}{1-t_1}\right)^j \left(\log \frac{1}{t_2}\right)^{r-\ell} \left(\log \frac{1}{1-u_1}\right)^{k-j} \left(\log \frac{1}{u_2}\right)^{\ell},$$

we see immediately the integral is separable, and by Proposition 1, its value is equal to

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^{j+\ell}\zeta(\{1\}^{j}, r-\ell+2)\zeta(\{1\}^{k-j}, \ell+2).$$

As a replacement of shuffle process, we decompose the region of integration into 6 simplices produced from all possible interlacing of variables t_1, t_2 and u_1, u_2. They are

(1) $D_1 : (t_1, t_2, u_1, u_2) \in [0, 1]^4, 0 < t_1 < t_2 < u_1 < u_2 < 1$,

(2) $D_2 : (t_1, t_2, u_1, u_2) \in [0, 1]^4, 0 < u_1 < u_2 < t_1 < t_2 < 1$,

(3) $D_3 : (t_1, t_2, u_1, u_2) \in [0, 1]^4, 0 < t_1 < u_1 < t_2 < u_2 < 1$,

(4) $D_4 : (t_1, t_2, u_1, u_2) \in [0, 1]^4, 0 < t_1 < u_1 < u_2 < t_2 < 1$,

(5) $D_5 : (t_1, t_2, u_1, u_2) \in [0, 1]^4, 0 < u_1 < t_1 < t_2 < u_2 < 1$ and

(6) $D_6 : (t_1, t_2, u_1, u_2) \in [0, 1]^4, 0 < u_1 < t_1 < u_2 < t_2 < 1$.

The integration over D_3, D_4, D_5 and D_6 are easily to get. For the simplex $D_3 : 0 < t_1 < u_1 < t_2 < u_2 < 1$, we rewrite the integral as

$$\frac{1}{k!r!}\int_{D_3}\frac{dt_1}{1-t_1}\left(\log\frac{1-t_1}{1-u_1}\right)^{k}\frac{du_1}{1-u_1}\frac{dt_2}{t_2}\left(\log\frac{u_2}{t_2}\right)^{r}\frac{du_2}{u_2}.$$

It comes from the Drinfeld integral

$$\int_0^1\prod_{j=1}^{k+2}\frac{dt_j}{1-t_j}\prod_{\ell=k+3}^{k+r+4}\frac{dt_\ell}{t_\ell}$$

and hence its value is $\zeta(\{1\}^{k+1}, r+3)$. A similar consideration leads to the values of the integrations over D_4, D_5 and D_6 are

$$(-1)^{r}\zeta(\{1\}^{k+1}, r+3),\ \ (-1)^{k}\zeta(\{1\}^{k+1}, r+3)\ \text{ and }\ \ (-1)^{k+r}\zeta(\{1\}^{k+1}, r+3),$$

respectively.

For the simplex $D_1 : 0 < t_1 < t_2 < u_1 < u_2 < 1$, we substitute the factor

$$\left(\log\frac{1-t_1}{1-u_1}\right)^{k}\quad\text{and}\quad\left(\log\frac{u_2}{t_2}\right)^{r}$$

by

$$\sum_{j=0}^{k} \binom{k}{j} \left(\log \frac{1-t_1}{1-t_2}\right)^{k-j} \left(\log \frac{1-t_2}{1-u_1}\right)^{j}$$

$$\text{and} \quad \sum_{\ell=0}^{r} \binom{r}{\ell} \left(\log \frac{u_1}{t_2}\right)^{\ell} \left(\log \frac{u_2}{u_1}\right)^{r-\ell}.$$

Consequently, in terms of multiple zeta values, the value of the integration over D_1 is

$$\sum_{j=0}^{k} \sum_{\ell=0}^{r} \sum_{|\boldsymbol{\alpha}|=j+\ell+1} \zeta(\{1\}^{k-j}, \alpha_0+1, \alpha_1, \ldots \alpha_j, r-\ell+2). \tag{2.1}$$

For $1 \leq j \leq k$, we have

$$\begin{aligned} &\sum_{|\boldsymbol{\alpha}|=j+\ell+1} \zeta(\{1\}^{k-j}, \alpha_0+1, \alpha_1, \ldots, \alpha_j, r-\ell+2) \\ &= \sum_{|\boldsymbol{\alpha}|=j+\ell+2} \zeta(\{1\}^{k-j}, \alpha_0, \alpha_1, \ldots, \alpha_j, r-\ell+2) \\ &\quad - \sum_{|\boldsymbol{\alpha}|=j+\ell+1} \zeta(\{1\}^{k-j+1}, \alpha_1, \ldots, \alpha_j, r-\ell+2), \end{aligned}$$

so that the sum in (2.1) is equal to

$$\sum_{\ell=0}^{r} \sum_{|\boldsymbol{\alpha}|=k+\ell+2} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, r-\ell+2).$$

Identifying $r-\ell+1$ as a new dummy variable, the above sum is

$$\sum_{|\boldsymbol{\alpha}|=k+r+3} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1) - \zeta(\{1\}^{k+1}, r+3).$$

Exchanging the roles of t_1, t_2 and u_1, u_2, the value of the integration over D_2 is

$$(-1)^{k+r} \left\{ \sum_{|\boldsymbol{\alpha}|=k+r+3} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1) - \zeta(\{1\}^{k+1}, r+3) \right\}.$$

Adding all the values we get from the integrations over $D_1, \ldots, D_6$, our assertion follows. $\square$

Remark 7. When $k+r$ is even, the sum formula

$$\sum_{|\boldsymbol{\alpha}|=k+r+3} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1) = \zeta(k+r+4)$$

is equivalent to the evaluation

$$\zeta(\{1\}^{k+1}, r+3) = (-1)^{k+1}\zeta(k+r+4) \\ + \frac{(-1)^k}{2} \sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{j+\ell} \zeta(\{1\}^j, r-\ell+2) \zeta(\{1\}^{k-j}, \ell+2).$$

To obtain the relation when the weight is odd, we consider the integral

$$\frac{1}{k!r!} \int_{0<t_1<t_2<1} \int_{0<u_1<u_2<1} \left(\log \frac{1-t_1}{1-u_1}\right)^k \left(\log \frac{u_2}{t_2}\right)^r \left(\log \frac{1}{u_2}\right) \\ \times \frac{dt_1 dt_2}{(1-t_1)t_2} \frac{du_1 du_2}{(1-u_1)u_2}$$

instead. Finally, we get the following relation

$$(-1)^{k+r}(r+1) \sum_{|\boldsymbol{\alpha}|=k+r+4} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1) \\ + \left\{1+(-1)^{k+r}\right\} \sum_{|\boldsymbol{\alpha}|=k+r+3} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+2) \\ + \left\{(-1)^k + (-1)^r(r+2)\right\} \zeta(\{1\}^{k+1}, r+4) \\ = \sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{j+\ell}(\ell+1) \zeta(\{1\}^j, r-\ell+2) \zeta(\{1\}^{k-j}, \ell+3).$$

In particular, when $k+r$ is even, we have

$$(r+1) \sum_{|\boldsymbol{\alpha}|=k+r+4} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1) \\ +2 \sum_{|\boldsymbol{\alpha}|=k+r+3} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+2) + (-1)^k(r+3)\zeta(\{1\}^{k+1}, r+4) \\ = \sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{j+\ell}(\ell+1) \zeta(\{1\}^j, r-\ell+2) \zeta(\{1\}^{k-j}, \ell+3).$$

Note that the second sum of multiple zeta values is equal to

$$2\sum_{\ell=0}^{r+1}\zeta(\ell+1,k+r-\ell+4)$$

by Ohno's generalization of the sum formula and the duality theorem.

The following proposition plays an important role in our proof of Theorem 4 and 5.

Proposition 8. *For a pair of integers k, $r \geq 0$ with k even, we have*

$$\sum_{|\boldsymbol{\alpha}|=k+r+3} 2^{\alpha_{k+1}}\zeta(\alpha_0,\alpha_1,\ldots,\alpha_k,\alpha_{k+1}+1) = \zeta(k+r+4)+\zeta(\{1\}^{k+1},r+3)$$
$$+\frac{1}{2}\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^j\zeta(\{1\}^j,r-\ell+2)\zeta(\{1\}^{k-j},\ell+2).$$

Proof. Consider the integral

$$\frac{1}{k!r!}\int_{0<t_1<t_2<1}\int_{0<u_1<u_2<1}\left(\log\frac{1-t_1}{1-u_1}\right)^k\left(\log\frac{1}{t_2}+\log\frac{1}{u_2}\right)^r$$
$$\times\frac{dt_1dt_2}{(1-t_1)t_2}\frac{du_1du_2}{(1-u_1)u_2}.$$

The above integral is separable and its value is given by

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^j\zeta(\{1\}^j,r-\ell+2)\zeta(\{1\}^{k-j},\ell+2).$$

Let D_j ($j=1,2,3,4,5,6$) be simplices obtained from all possible interlacing of variables t_1,t_2 and u_1,u_2. Note that the integrand of the integral is invariant if we exchange the roles of t_1,t_2 and u_1,u_2. Therefore, it suffices to evaluate the integration over $D_1: 0<t_1<t_2<u_1<u_2<1$, $D_3: 0<t_1<u_1<t_2<u_2<1$ and $D_4: 0<t_1<u_1<u_2<t_2<1$.

For the simplex D_1, we rewrite the integral as

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}\frac{1}{j!(k-j)!\ell!(r-\ell)!}\int_{D_1}\frac{dt_1}{1-t_1}\left(\log\frac{1-t_1}{1-t_2}\right)^{k-j}$$
$$\times\frac{dt_2}{t_2}\left(\log\frac{1-t_2}{1-u_1}\right)^j\left(\log\frac{u_1}{t_2}\right)^\ell\frac{du_1}{1-u_1}\left(\log\frac{u_2}{u_1}+2\log\frac{1}{u_2}\right)^{r-\ell}\frac{du_2}{u_2}.$$

In terms of multiple zeta values, it is equal to

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}(2^{r-\ell+1}-1)\sum_{|\boldsymbol{\alpha}|=j+1+\ell}\zeta(\{1\}^{k-j}, \alpha_0+1, \alpha_1, \ldots, \alpha_j, r-\ell+2).$$

Sum over k leads to

$$\sum_{\ell=0}^{r}(2^{r-\ell+1}-1)\sum_{|\boldsymbol{\alpha}|=k+\ell+2}\zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, r-\ell+2).$$

Identifying $r-\ell+1$ as a new variable α_{k+1}, it is

$$\sum_{|\boldsymbol{\alpha}|=k+r+3}(2^{\alpha_{k+1}}-1)\zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1)-(2^{r+2}-1)\zeta(\{1\}^{k+1}, r+3).$$

Both the integrations over D_3 and D_4 have the same value

$$(2^{r+1}-1)\zeta(\{1\}^{k+1}, r+3).$$

Including the integrations over D_2, D_5 and D_6, we get the identity

$$\begin{aligned}&2\sum_{|\boldsymbol{\alpha}|=k+r+3}(2^{\alpha_{k+1}}-1)\zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1)-2\zeta(\{1\}^{k+1}, r+3)\\ &=\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^j\zeta(\{1\}^j, r-\ell+2)\zeta(\{1\}^{k-j}, \ell+2).\end{aligned}$$

Thus our assertion follows from the sum formula. $\square$

3 The proof of Theorem 4

In our previous considerations, the integrands are so simple that it is easy to evaluate the integrations over all the simplices D_j $(j=1,2,3,4,5,6)$. It will be a different story for our next consideration. For our convenience, we shall use the notation

$$\zeta(\boldsymbol{\alpha}, m)=\zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, m).$$

Now we are ready to prove Theorem 4.

Proof of Theorem 4. For a pair of integers $k,\ r \geq 0$, we consider the integral

$$\frac{1}{k!r!}\int_{0<t_1<t_2<1}\int_{0<u_1<u_2<1}\left(\log\frac{1-t_1}{1-u_1}\right)^k\left(\log\frac{u_2}{t_1}+\log\frac{u_2}{u_1}\right)^r \times\frac{dt_1dt_2}{(1-t_1)t_2}\frac{du_1du_2}{(1-u_1)u_2}.$$

Rewrite the second factor in the integrand as

$$\sum_{\ell=0}^{r}\binom{r}{\ell}\left(\log\frac{1}{t_1}\right)^{r-\ell}\left(\log\frac{u_2}{u_1}-\log\frac{1}{u_2}\right)^{\ell}.$$

Also we have

$$\begin{aligned}
&\frac{1}{j!(r-\ell)!}\int_{0<t_1<t_2<1}\left(\log\frac{1}{1-t_1}\right)^j\left(\log\frac{1}{t_1}\right)^{r-\ell}\frac{dt_1dt_2}{(1-t_1)t_2}\\
&=\sum_{p+q=r-\ell}\frac{1}{j!p!q!}\int_{0<t_1<t_2<1}\left(\log\frac{1}{1-t_1}\right)^j\left(\log\frac{t_2}{t_1}\right)^p\left(\log\frac{1}{t_2}\right)^q\frac{dt_1dt_2}{(1-t_1)t_2}\\
&=\sum_{p+q=r-\ell}\zeta(\{1\}^j,p+q+2)=(r-\ell+1)\zeta(\{1\}^j,r-\ell+2)
\end{aligned}$$

and

$$\begin{aligned}
&\frac{1}{(k-j)!\ell!}\int_{0<u_1<u_2<1}\left(\log\frac{1}{1-u_1}\right)^{k-j}\left(\log\frac{u_2}{u_1}-\log\frac{1}{u_2}\right)^{\ell}\frac{du_1du_2}{(1-u_1)u_2}\\
&=\sum_{p+q=\ell}\frac{(-1)^q}{(k-j)!p!q!}\int_{0<u_1<u_2<1}\left(\log\frac{1}{1-u_1}\right)^{k-j}\left(\log\frac{u_2}{u_1}\right)^p\left(\log\frac{1}{u_2}\right)^q\\
&\qquad\times\frac{du_1du_2}{(1-u_1)u_2}=\sum_{p+q=\ell}(-1)^q\zeta(\{1\}^{k-j},p+q+2)\\
&=\frac{1+(-1)^{\ell}}{2}\zeta(\{1\}^{k-j},\ell+2).
\end{aligned}$$

Consequently, the integral is separable and its value is given by

$$\begin{aligned}
&\frac{1}{2}\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^j(r-\ell+1)\zeta(\{1\}^j,r-\ell+2)\zeta(\{1\}^{k-j},\ell+2)\\
&+\frac{1}{2}\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^{j+\ell}(r-\ell+1)\zeta(\{1\}^j,r-\ell+2)\zeta(\{1\}^{k-j},\ell+2).
\end{aligned}$$

When both k and r are even, the above sum is equal to

$$\frac{r+2}{4}\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^j\zeta(\{1\}^j, r-\ell+2)\zeta(\{1\}^{k-j}, \ell+2)$$
$$+\frac{r+2}{4}\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^{j+\ell}\zeta(\{1\}^j, r-\ell+2)\zeta(\{1\}^{k-j}, \ell+2).$$

The sum of the second summation, by Proposition 6, is equal to

$$\frac{r+2}{2}\left\{\zeta(k+r+4)+\zeta(\{1\}^{k+1}, r+3)\right\}$$

and hence the total is

$$\frac{r+2}{2}\sum_{|\boldsymbol{\alpha}|=k+r+3} 2^{\alpha_{k+1}}\zeta(\alpha_0,\alpha_1,\ldots,\alpha_k,\alpha_{k+1}+1)$$

by Proposition 8.

Next we evaluate the integrations over D_j ($j = 1,2,3,4,5,6$). For the simplex $D_1 : 0 < t_1 < t_2 < u_1 < u_2 < 1$, we rewrite the integral as

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}\sum_{a+b=\ell}\frac{1}{j!(k-j)!a!b!(r-\ell)!}\int_{D_1}\frac{dt_1}{1-t_1}\left(\log\frac{1-t_1}{1-t_2}\right)^j\left(\log\frac{t_2}{t_1}\right)^a\frac{dt_2}{t_2}$$
$$\times\left(\log\frac{1-t_2}{1-u_1}\right)^{k-j}\left(\log\frac{u_1}{t_2}\right)^b\frac{du_1}{1-u_1}\left(2\log\frac{u_2}{u_1}\right)^{r-\ell}\frac{du_2}{u_2},$$

so it can be expressed as

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}2^{r-\ell}\sum_{a+b=\ell}\sum_{\substack{|\boldsymbol{\alpha}|=j+1+a\\|\boldsymbol{\beta}|=k-j+1+b}}\zeta(\alpha_0,\alpha_1,\ldots,\alpha_j+\beta_j,\beta_{j+1},\ldots,\beta_k, r-\ell+2)$$

or

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}2^{r-\ell}\sum_{|\boldsymbol{\alpha}|=k+\ell+2}(\alpha_j-1)\zeta(\boldsymbol{\alpha}, r-\ell+2).$$

For fixed ℓ, by counting the number of $\zeta(\alpha_0,\alpha_1,\ldots,\alpha_k, r-\ell+2)$ appeared in the summation, we conclude that the sum is equal to

$$\sum_{\ell=0}^{r}2^{r-\ell}(\ell+1)\sum_{|\boldsymbol{\alpha}|=k+\ell+2}\zeta(\boldsymbol{\alpha}, r-\ell+2).$$

Extending the above sum to $\ell = -1$ and then set $\ell + 1$ as a new dummy variable, the sum is

$$(r+1) \sum_{|\boldsymbol{\alpha}|=k+r+2} \zeta(\boldsymbol{\alpha}, 2) + \sum_{\ell=0}^{r} 2^{r-\ell+1} \ell \sum_{|\boldsymbol{\alpha}|=k+\ell+1} \zeta(\boldsymbol{\alpha}, r-\ell+3).$$

The integration over D_2 is just the alternating double sum

$$\sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{\ell} \sum_{\substack{|\boldsymbol{\alpha}|=j+r-\ell+1 \\ |\boldsymbol{\beta}|=k-j+\ell+1}} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_j + \beta_j, \beta_{j+1}, \ldots, \beta_k, 2)$$

which would be denoted by G in the after.

The integrations over D_3, D_4, D_5 and D_6 yield the following multiple zeta values

$$\sum_{\ell=0}^{r} 2^{r-\ell}(r-\ell+1) \sum_{|\boldsymbol{\alpha}|=k+\ell+1} \zeta(\boldsymbol{\alpha}, r-\ell+3), \quad \sum_{\ell=0}^{r} 2^{r-\ell} \sum_{|\boldsymbol{\alpha}|=k+\ell+1} \zeta(\boldsymbol{\alpha}, r-\ell+3),$$

$$\sum_{\ell=0}^{r} 2^{r-\ell}(r-\ell+1) \sum_{|\boldsymbol{\alpha}|=k+\ell+1} \zeta(\boldsymbol{\alpha}, r-\ell+3) \text{ and } \sum_{\ell=0}^{r} 2^{r-\ell} \sum_{|\boldsymbol{\alpha}|=k+\ell+1} \zeta(\boldsymbol{\alpha}, r-\ell+3).$$

Adding together all the values obtained from the integrations over the simplices D_j ($j = 1, 2, 3, 4, 5, 6$), we get the identity

$$\begin{aligned}
&(r+1) \sum_{|\boldsymbol{\alpha}|=k+r+2} \zeta(\boldsymbol{\alpha}, 2) + (r+2) \sum_{\ell=0}^{r} 2^{r-\ell+1} \sum_{|\boldsymbol{\alpha}|=k+\ell+1} \zeta(\boldsymbol{\alpha}, r-\ell+3) \\
&\quad + \sum_{j=0}^{k} \sum_{\ell=0}^{r} (-1)^{\ell} \sum_{\substack{|\boldsymbol{\alpha}|=j+r-\ell+1 \\ |\boldsymbol{\beta}|=k-j+\ell+1}} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_j + \beta_j, \beta_{j+1}, \ldots, \beta_k, 2) \\
&= \frac{r+2}{2} \sum_{|\boldsymbol{\alpha}|=k+r+3} 2^{\alpha_{k+1}} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1).
\end{aligned}$$

Our assertion follows from

$$\begin{aligned}
&\sum_{|\boldsymbol{\alpha}|=k+r+3} 2^{\alpha_{k+1}} \zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, \alpha_{k+1}+1) \\
&= 2 \sum_{|\boldsymbol{\alpha}|=k+r+2} \zeta(\boldsymbol{\alpha}, 2) + 2 \sum_{\ell=0}^{r} 2^{r-\ell+1} \sum_{|\boldsymbol{\alpha}|=k+\ell+1} \zeta(\boldsymbol{\alpha}, r-\ell+3). \qquad \square
\end{aligned}$$

On the other hand, if we consider the integral

$$\frac{1}{k!r!}\int_{0<t_1<t_2<1}\int_{0<u_1<u_2<1}\left(\log\frac{1-t_1}{1-u_1}\right)^k\left(\log\frac{u_2}{t_2}+\log\frac{u_2}{u_1}\right)^r \times\frac{dt_1dt_2}{(1-t_1)t_2}\frac{du_1du_2}{(1-u_1)u_2},$$

it has the value

$$\frac{1}{2}\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^j(1+(-1)^\ell)\zeta(\{1\}^j, r-\ell+2)\zeta(\{1\}^{k-j}, \ell+2).$$

The assertion in Theorem 5 follows after a similar procedure.

4 A final remark

Through the double generating function

$$\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\zeta(\{1\}^m, n+2)x^{n+1}y^{m+1} = 1-\exp\left\{\sum_{k=2}^{\infty}\left(x^k+y^k-(x+y)^k\right)\frac{\zeta(k)}{k}\right\},$$

we are able to express $\zeta(\{1\}^m, n+2)$ in terms of the special values of Riemann zeta function at positive integers. The shuffle relations in Proposition 6 provide us to evaluate $\zeta(\{1\}^m, n+2)$ recursively in terms of special values of Riemann zeta function.

Another way to prove Theorem 4 is to count the number of appearances of each $\zeta(\alpha_0, \alpha_1, \ldots, \alpha_k, 2)$ in the complicated double alternating sum. Therefore the identity is just a problem of counting and can be extended. For example, for a pair of even integers $k, r \geq 0$, we have

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^\ell\sum_{\substack{|\boldsymbol{\alpha}|=j+r-\ell+1\\|\boldsymbol{\beta}|=k-j+\ell+1}}\zeta(\alpha_0, \alpha_1, \ldots, \alpha_j+\beta_j, \beta_{j+1}, \ldots, \beta_k+1)$$

$$= \sum_{|\boldsymbol{\alpha}|=k+r+2}\zeta(\alpha_0, \alpha_1, \ldots, \alpha_k+1) = \zeta(k+r+3)$$

or for any positive integer $m \geq 2$,

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^{\ell}\sum_{\substack{|\boldsymbol{\alpha}|=j+r-\ell+1\\|\boldsymbol{\beta}|=k-j+\ell+1}}\zeta(\alpha_0,\alpha_1,\ldots,\alpha_j+\beta_j,\beta_{j+1},\ldots,\beta_k,m)$$
$$=\sum_{|\boldsymbol{\alpha}|=k+r+2}\zeta(\alpha_0,\alpha_1,\ldots,\alpha_k,m)$$

or for a string of nonnegative integers $p_0, p_1, \cdots, p_k$

$$\sum_{j=0}^{k}\sum_{\ell=0}^{r}(-1)^{\ell}\sum_{\substack{|\boldsymbol{\alpha}|=j+r-\ell+1\\|\boldsymbol{\beta}|=k-j+\ell+1}}\zeta(\alpha_0+p_0,\alpha_1+p_1,\ldots,\alpha_j+\beta_j+p_j,\ldots,$$
$$\ldots,\beta_k+p_k+1) = \sum_{|\boldsymbol{\alpha}|=k+r+2}\zeta(\alpha_0+p_0,\alpha_1+p_1,\ldots,\alpha_k+p_k+1).$$

All these identities are difficult to be proved otherwise.

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