

DUALITY/SUM FORMULAS FOR ITERATED INTEGRALS AND THEIR APPLICATION TO MULTIPLE ZETA VALUES

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ABSTRACT. We investigate linear relations among a class of iterated integrals on the Riemann sphere minus four points $0, 1, z$ and ∞ . Generalization of the duality formula and the sum formula for multiple zeta values to the iterated integrals are given.

1. INTRODUCTION AND MAIN RESULTS

The multiple zeta value, originally considered by Euler [3], is defined for positive integers k_1, \dots, k_r with $k_r \geq 2$ by

$$\zeta(k_1, \dots, k_r) = \sum_{0 < m_1 < \dots < m_r} \frac{1}{m_1^{k_1} \dots m_r^{k_r}}.$$

These real numbers satisfy numerous linear relations over \mathbb{Q} and have been studied in recent years by many mathematicians and physicists (see [2, 5, 11, 13, 16] for example), but their structure is not completely understood at the time of writing.

In this paper we present a new approach to linear relations among multiple zeta values through a study of linear relations among the iterated integrals on $\mathbb{P}^1 \setminus \{0, 1, z, \infty\}$ with a complex variable $z \in \mathbb{C} \setminus [0, 1]$:

$$I(0; a_1, \dots, a_n; 1) = \int_0^1 \frac{dt_n}{t_n - a_n} \int_0^{t_n} \frac{dt_{n-1}}{t_{n-1} - a_{n-1}} \dots \int_0^{t_2} \frac{dt_1}{t_1 - a_1} \quad (a_1, \dots, a_n \in \{0, 1, z\}).$$

We assume $a_1 \neq 0$ and $a_n \neq 1$ for the convergence of the integral. Since the iterated integral $I(0; a_1, \dots, a_n; 1)$ is a holomorphic function of z , we may use analytic methods to obtain relations among these iterated integrals. In fact, a formula for the differentiation of $I(0; a_1, \dots, a_n; 1)$ with respect to z (Theorem 2.1; see also [4, Theorem 2.1]) is useful to prove linear relations. Moreover, using the iterated integral expression

$$\zeta(k_1, \dots, k_r) = (-1)^r I(0; 1, \overbrace{0, \dots, 0}^{k_1-1}, \dots, 1, \overbrace{0, \dots, 0}^{k_r-1}; 1) \quad (1.1)$$

of multiple zeta values due to Kontsevich and Drinfeld, one may obtain linear relations among multiple zeta values as a specialization of linear relations among $I(0; a_1, \dots, a_n; 1)$'s.

2010 *Mathematics Subject Classification*. Primary 11M32, Secondary 11F67, 33E20.

Key words and phrases. Iterated integrals, Multiple zeta values.

With this approach, we rediscover the so-called duality formula and the sum formula satisfied by multiple zeta values as a specialization of the linear relation among the iterated integrals obtained in this paper (Theorems 1.1 and 1.2). Our ultimate goal is to capture all linear relations among the iterated integral. This will be developed minutely in the upcoming paper [7] (see also [8]).

Let us formulate our main results. It is convenient to use the algebraic setup given by Hoffman [10] for multiple zeta values. Let $\mathcal{A} = \mathbb{Q}\langle e_0, e_1, e_z \rangle$ be the non-commutative polynomial algebra over \mathbb{Q} in three indeterminate elements e_0, e_1 and e_z , and \mathcal{A}^0 be its linear subspace $\mathbb{Q} + \mathbb{Q}e_z + e_z\mathcal{A}e_z + e_z\mathcal{A}e_0 + e_1\mathcal{A}e_z + e_1\mathcal{A}e_0$. We also denote by L the \mathbb{Q} -linear map that assigns the iterated integral $I(0; a_1, a_2, \dots, a_n; 1)$ to a word $e_{a_1}e_{a_2} \cdots e_{a_n}$ in \mathcal{A}^0 , which by definition converges absolutely. For example, by (1.1) we have $L(e_1e_0^{k_1-1} \cdots e_1e_0^{k_r-1}) = (-1)^r \zeta(k_1, \dots, k_r)$.

Our duality formula is stated as follows.

Theorem 1.1 (Duality formula). *Let τ be the anti-automorphism on \mathcal{A} (i.e., $\tau(xy) = \tau(y)\tau(x)$) holds for $x, y \in \mathcal{A}$) given by*

$$\tau(e_0) = e_z - e_1, \quad \tau(e_1) = e_z - e_0, \quad \tau(e_z) = e_z.$$

Then, for any $w \in \mathcal{A}^0$, we obtain

$$L(w - \tau(w)) = 0. \tag{1.2}$$

Our derivation of the formula (1.2) can be regarded as an application of Okuda's result ([13, Theorem 4.2]). Thanks to the existence of a special Möbius transformation on \mathbb{P}^1 which preserves the subset $\{0, 1, z, \infty\}$, we could derive the equality (1.2). Taking $z \rightarrow \infty$ in (1.2), we can recover the duality formula for multiple zeta values [16, Section 9] (see also [9]):

$$I(0; a_1, \dots, a_n; 1) = (-1)^n I(0; 1 - a_n, \dots, 1 - a_1; 1) \quad (a_1, \dots, a_n \in \{0, 1\}). \tag{1.3}$$

On the other hand, setting $z = -1$ in (1.2), we can also derive the Broadhurst duality (see [1, eq. (127)], [13, Example 4.2] and [2, Section 4]), which is known as a family of \mathbb{Q} -linear relations among alternating Euler sums.

Our sum formula is stated as follows.

Theorem 1.2 (Sum formula). *For any integers k, r satisfying $k \geq 2$ and $k \geq r \geq 1$, we have*

$$\begin{aligned} & (-1)^r \sum_{\substack{k_1 + \cdots + k_r = k \\ k_i \geq 1, \ k_r \geq 2}} L(e_z e_0^{k_1-1} e_1 e_0^{k_2-1} \cdots e_1 e_0^{k_r-1}) \\ &= -L(e_1 e_0^{k-1}) + L((e_1 - e_z)(e_0 - e_z)^{r-1} e_0^{k-r}). \end{aligned} \tag{1.4}$$

We remark that, taking the limit $z \rightarrow 1 + 0$, the above formula is reduced to the following sum formula for multiple zeta values: For any integers $k > r > 1$, we can take the limit in the both hand sides of (1.4) and we obtain

$$\sum_{\substack{k_1 + \dots + k_r = k \\ k_i \geq 1, \ k_r \geq 2}} \zeta(k_1, \dots, k_r) = \zeta(k). \quad (1.5)$$

This formula was first proved by Granville [6] and Zagier (see also [9, §3]) independently. Our method gives a new proof of (1.5).

Here we briefly illustrate a few examples of relations, which might be useful to understand the strategy of our proof. As special cases of Theorem 1.2, we will prove

$$I(0; z, 1, 0; 1) + I(0; 1, z, 0; 1) + I(0; z, 0, 0; 1) - I(0; z, z, 0; 1) = 0 \quad (1.6)$$

for the case $(k, r) = (3, 2)$, and

$$I(0; z, z; 1) - I(0; z, 0; 1) - I(0; 1, z; 1) = 0 \quad (1.7)$$

for the case $(k, r) = (2, 2)$. We can show that the equality (1.6) can be obtained by integrating both sides of (1.7). (Integration constants can be determined by considering the limit $z \rightarrow \infty$). This is a consequence of a formula describing the differentiation of the iterated integrals with respect to z (Theorem 2.1). In general, we can check that the differentiation reduces the value of k or r in the desired formula (1.4), and hence a proof by induction works perfectly. The differential formula plays an essential role here, and it is the main advantage to consider the iterated integral with a complex variable z .

This paper is organized as follows. In Section 2 we fix notations and give a proof of the formula for differentiation of the iterated integrals with respect to z (Theorem 2.1). This differential formula can be regarded as a special case of [4, Theorem 2.1]. We give another proof of the fact. Section 3 is devoted to proofs of our main theorems along the ideas presented above.

ACKNOWLEDGEMENTS

The authors would like to thank Erik Panzer for his useful comments. This work was partially supported by JSPS KAKENHI Grant Number 16H07115, 16H06337 and 16K17613.

2. ITERATED INTEGRALS WITH A COMPLEX VARIABLE AND THE DIFFERENTIAL FORMULA

2.1. Definitions and notations. In this paper we assume that $z \in \mathbb{C} \setminus [0, 1]$. For any $a_1, \dots, a_n \in \{0, 1, z\}$ satisfying $a_1 \neq 0$ and $a_n \neq 1$ we use the standard notation

$I(0; a_1, \dots, a_n; 1)$ for the iterated integral:

$$\begin{aligned} I(0; a_1, \dots, a_n; 1) &:= \int_{0 < t_1 < t_2 < \dots < t_n < 1} \prod_{i=1}^n \frac{dt_i}{t_i - a_i} \\ &= \int_0^1 \frac{dt_n}{t_n - a_n} \int_0^{t_n} \frac{dt_{n-1}}{t_{n-1} - a_{n-1}} \dots \int_0^{t_2} \frac{dt_1}{t_1 - a_1}. \end{aligned} \quad (2.1)$$

The above iterated integral is called the hyperlogarithm which was introduced long ago (e.g., [12]), and has been studied by many mathematicians and physicists (see, [1, 15, 5] for example). As a function of z , the iterated integral $I(0; a_1, \dots, a_n; 1)$ is a (single-valued) holomorphic function on the domain $\mathbb{C} \setminus [0, 1]$, and $\lim_{z \rightarrow \infty} I(0; a_1, \dots, a_n; 1) = 0$ holds if $z \in \{a_1, \dots, a_n\}$. The \mathbb{Q} -linear space spanned by iterated integrals of such a form is denoted by

$$\mathcal{Z}^{(z)} := \langle I(0; a_1, \dots, a_n; 1) \mid n \geq 0, a_i \in \{0, 1, z\}, a_1 \neq 0, a_n \neq 1 \rangle_{\mathbb{Q}}.$$

Let $\mathcal{A} := \mathbb{Q}\langle e_0, e_1, e_z \rangle$ be the non-commutative polynomial algebra of words consisting of three letters e_0, e_1, e_z , and

$$\mathcal{A}^0 := \mathbb{Q} + \mathbb{Q}e_z + e_z\mathcal{A}e_z + e_z\mathcal{A}e_0 + e_1\mathcal{A}e_z + e_1\mathcal{A}e_0$$

the subalgebra of convergent words. We also define a \mathbb{Q} -linear map $L : \mathcal{A}^0 \rightarrow \mathcal{Z}^{(z)}$ by

$$L(1) := 1, \quad L(e_{a_1}e_{a_2} \dots e_{a_n}) := I(0; a_1, a_2, \dots, a_n; 1).$$

2.2. Differential formula for the iterated integrals. For any convergent word $w \in \mathcal{A}^0$, we regard the corresponding iterated integral $L(w)$ as a holomorphic function of z on the domain $\mathbb{C} \setminus [0, 1]$. Here we show a formula which describes the differentiation of the iterated integral with respect to z . The formula is quite useful in the proof of our main result.

For convenience, we write $a_0 = 0$ and $a_{n+1} = 1$ throughout this paper. For $x, y \in \{0, 1, z\}$, we define a \mathbb{Q} -linear map $\partial_{x,y} : \mathcal{A}^0 \rightarrow \mathcal{A}^0$ by

$$\partial_{x,y}(1) := 0, \quad \partial_{x,y}(e_{a_1} \dots e_{a_n}) := \sum_{i=1}^n (\delta_{\{a_i, a_{i+1}\}, \{x,y\}} - \delta_{\{a_{i-1}, a_i\}, \{x,y\}}) e_{a_1} \dots \widehat{e_{a_i}} \dots e_{a_n},$$

where

$$\delta_{\{a,b\}, \{x,y\}} := \begin{cases} 1 & \text{if } \{a, b\} = \{x, y\} \text{ as subsets of } \{0, 1, z\} \\ 0 & \text{otherwise.} \end{cases}$$

It is easy to check that $\partial_{x,y}$ is well-defined. Then we have the following theorem.

Theorem 2.1 (Differential formula (c.f., [4, Theorem 2.1] and [15, Lemma 3.3.30])). *For any $w \in \mathcal{A}^0$, we have*

$$\frac{d}{dz}L(w) = \sum_{a \in \{0,1\}} \frac{1}{z-a} L(\partial_{z,a}w). \quad (2.2)$$

The above formula can be regarded as a special case of a result obtained in [15]. Here we propose an alternative proof of (2.2) for any convergent word $w = e_{a_1} \cdots e_{a_n} \in \mathcal{A}^0$. We also note that [4] proved the formula as well when each consecutive letters e_{a_i} and $e_{a_{i+1}}$ in w are distinct.

The claim for $n = 0$ is obvious. For $n = 1$, the equality (2.2) is easily checked as

$$\frac{d}{dz}L(e_z) = \int_0^1 \frac{dt}{(t-z)^2} = -\frac{1}{z} + \frac{1}{z-1}.$$

Let us assume that $n \geq 2$.

Lemma 2.2. (1) *For any convergent word $w = e_{a_1} \cdots e_{a_n} \in \mathcal{A}^0$, we have*

$$\frac{d}{dz}L(w) = \sum_{\substack{1 \leq i \leq n \\ a_i = z}} J_{i-1}(a_0, \dots, a_{n+1}) - \sum_{\substack{1 \leq i \leq n \\ a_i = z}} J_i(a_0, \dots, a_{n+1}),$$

where, for given $0 \leq i \leq n$, we put

$$J_i(a_0, \dots, a_{n+1}) := \begin{cases} \frac{1}{a_0 - a_1} L(\widehat{e_{a_1}} e_{a_2} \cdots e_{a_n}) & \text{if } i = 0, \\ \int_{a_0 < t_1 < \cdots < t_i < t_{i+2} < \cdots < t_n < a_{n+1}} \frac{dt_i}{(t_i - a_i)(t_i - a_{i+1})} \prod_{\substack{j=1 \\ j \neq i, i+1}}^n \frac{dt_j}{t_j - a_j} & \text{if } 1 \leq i \leq n-1, \\ -\frac{1}{a_n - a_{n+1}} L(e_{a_1} \cdots e_{a_{n-1}} \widehat{e_{a_n}}) & \text{if } i = n. \end{cases}$$

Here we regard the domain of the integration in the definition of $J_{n-1}(a_0, \dots, a_{n+1})$ as $\{(t_1, \dots, t_{n-1}) \in \mathbb{R}^{n-1} \mid a_0 < t_1 < \cdots < t_{n-1} < a_{n+1}\}$.

(2) *For $1 \leq i \leq n-1$ with $a_i \neq a_{i+1}$, we have*

$$J_i(a_0, \dots, a_{n+1}) = \frac{1}{a_i - a_{i+1}} \{L(e_{a_1} \cdots \widehat{e_{a_{i+1}}} \cdots e_{a_n}) - L(e_{a_1} \cdots \widehat{e_{a_i}} \cdots e_{a_n})\}. \quad (2.3)$$

Proof. Differentiating $L(w) = I(a_0; a_1, \dots, a_n; a_{n+1})$ with respect to z , we have

$$\frac{d}{dz}L(w) = \frac{da_1}{dz} \int_{a_0 < t_2 < \cdots < t_n < a_{n+1}} \left(\prod_{j=2}^n \frac{dt_j}{t_j - a_j} \right) \left(\int_{a_0}^{t_2} \frac{dt_1}{(t_1 - a_1)^2} \right)$$

$$\begin{aligned}
& + \sum_{i=2}^{n-1} \frac{da_i}{dz} \int_{a_0 < t_1 < \dots < t_{i-1} < t_{i+1} < \dots < t_n < a_{n+1}} \left(\prod_{\substack{j=1 \\ j \neq i}}^n \frac{dt_j}{t_j - a_j} \right) \left(\int_{t_{i-1}}^{t_{i+1}} \frac{dt_i}{(t_i - a_i)^2} \right) \\
& + \frac{da_n}{dz} \int_{a_0 < t_1 < \dots < t_{n-1} < a_{n+1}} \left(\prod_{j=1}^{n-1} \frac{dt_j}{t_j - a_j} \right) \left(\int_{t_{n-1}}^{a_{n+1}} \frac{dt_n}{(t_n - a_n)^2} \right). \tag{2.4}
\end{aligned}$$

The first line in the right-hand side of (2.4) can be reduced to

$$\begin{aligned}
& \frac{da_1}{dz} \int_{a_0 < t_2 < \dots < t_n < a_{n+1}} \left(\prod_{j=2}^n \frac{dt_j}{t_j - a_j} \right) \left(\int_{a_0}^{t_2} \frac{dt_1}{(t_1 - a_1)^2} \right) \\
& = \frac{da_1}{dz} \int_{a_0 < t_2 < \dots < t_n < a_{n+1}} \left(\prod_{j=2}^n \frac{dt_j}{t_j - a_j} \right) \left(\frac{1}{a_0 - a_1} - \frac{1}{t_2 - a_1} \right) \\
& = \frac{da_1}{dz} (J_0(a_0, \dots, a_{n+1}) - J_1(a_0, \dots, a_{n+1})).
\end{aligned}$$

By a similar computation, the second and the third lines in (2.4) are reduced to

$$\sum_{i=1}^{n-1} \frac{da_i}{dz} (J_{i-1}(a_0, \dots, a_{n+1}) - J_i(a_0, \dots, a_{n+1}))$$

and

$$\frac{da_n}{dz} (J_{n-1}(a_0, \dots, a_{n+1}) - J_n(a_0, \dots, a_{n+1})),$$

respectively. Thus we have proved (1).

The claim (2) follows from the partial fraction decomposition

$$\frac{dt_i}{(t_i - a_i)(t_i - a_{i+1})} = \frac{1}{a_i - a_{i+1}} \left(\frac{dt_i}{t_i - a_i} - \frac{dt_i}{t_i - a_{i+1}} \right).$$

□

Proof of Theorem 2.1. The claim (1) of Lemma 2.2 implies

$$\frac{d}{dz} L(w) = S_1 + S_2,$$

where

$$S_1 = \sum_{\substack{1 \leq i \leq n \\ a_i = z}} J_{i-1}(a_0, \dots, a_{n+1}), \quad S_2 = - \sum_{\substack{1 \leq i \leq n \\ a_i \neq z}} J_i(a_0, \dots, a_{n+1})$$

We divide S_1 (resp., S_2) as $S_1 = S_1^{(\text{I})} + S_1^{(\text{II})}$ (resp., $S_2 = S_2^{(\text{I})} + S_2^{(\text{II})}$), where

$$S_1^{(\text{I})} = \sum_{\substack{1 \leq i \leq n \\ a_{i-1} = a_i = z}} J_{i-1}(a_0, \dots, a_{n+1}), \quad S_1^{(\text{II})} = \sum_{\substack{1 \leq i \leq n \\ a_{i-1} \neq a_i = z}} J_{i-1}(a_0, \dots, a_{n+1}), \tag{2.5}$$

$$S_2^{(\text{I})} = - \sum_{\substack{1 \leq i \leq n \\ a_i = a_{i+1} = z}} J_i(a_0, \dots, a_{n+1}), \quad S_2^{(\text{II})} = - \sum_{\substack{1 \leq i \leq n \\ a_{i+1} \neq a_i = z}} J_i(a_0, \dots, a_{n+1}). \quad (2.6)$$

Since $a_0, a_{n+1} \neq z$, $S_1^{(\text{I})}$ and $S_2^{(\text{I})}$ can also be expressed as

$$S_1^{(\text{I})} = \sum_{\substack{2 \leq i \leq n \\ a_{i-1} = a_i = z}} J_{i-1}(a_0, \dots, a_{n+1}), \quad S_2^{(\text{I})} = - \sum_{\substack{1 \leq i \leq n-1 \\ a_i = a_{i+1} = z}} J_i(a_0, \dots, a_{n+1})$$

Therefore, $S_1^{(\text{I})} + S_2^{(\text{I})}$ vanishes identically. On the other hand, using (2.3) we obtain

$$\begin{aligned} S_1^{(\text{II})} &= \sum_{\substack{1 \leq i \leq n \\ a_{i-1} \neq z, a_i = z}} \frac{1}{a_{i-1} - z} L(e_{a_1} \cdots \widehat{e_{a_i}} \cdots e_{a_n}) - \sum_{\substack{1 \leq i \leq n \\ a_i \neq z, a_{i+1} = z}} \frac{1}{a_i - z} L(e_{a_1} \cdots \widehat{e_{a_i}} \cdots e_{a_n}) \\ &= \sum_{b \in \{0,1\}} \frac{1}{z - b} L \left(\sum_{1 \leq i \leq n} (-\delta_{(a_{i-1}, a_i), (b, z)} + \delta_{(a_i, a_{i+1}), (b, z)}) e_{a_1} \cdots \widehat{e_{a_i}} \cdots e_{a_n} \right). \end{aligned} \quad (2.7)$$

and

$$\begin{aligned} S_2^{(\text{II})} &= - \sum_{\substack{1 \leq i \leq n \\ a_{i-1} = z, a_i \neq z}} \frac{1}{z - a_i} L(e_{a_1} \cdots \widehat{e_{a_i}} \cdots e_{a_n}) + \sum_{\substack{1 \leq i \leq n \\ a_i = z, a_{i+1} \neq z}} \frac{1}{z - a_{i+1}} L(e_{a_1} \cdots \widehat{e_{a_i}} \cdots e_{a_n}) \\ &= \sum_{b \in \{0,1\}} \frac{1}{z - b} L \left(\sum_{1 \leq i \leq n} (-\delta_{(a_{i-1}, a_i), (z, b)} + \delta_{(a_i, a_{i+1}), (z, b)}) e_{a_1} \cdots \widehat{e_{a_i}} \cdots e_{a_n} \right) \end{aligned} \quad (2.8)$$

respectively, where we put

$$\delta_{(a,b), (x,y)} := \begin{cases} 1 & \text{if } a = x \text{ and } b = y \\ 0 & \text{otherwise.} \end{cases}$$

Therefore, since $\delta_{\{a,b\}, \{x,y\}} = \delta_{(a,b), (x,y)} + \delta_{(a,b), (y,x)}$ for $x \neq y$, summing up (2.7) and (2.8), we obtain

$$\frac{d}{dz} L(e_{a_1} \cdots e_{a_n}) = \sum_{b \in \{0,1\}} \frac{1}{z - b} L(\partial_{z,b}(e_{a_1} \cdots e_{a_n}))$$

which proves (2.2) for $n \geq 2$. This completes the proof of Theorem 2.1. \square

Example 2.3. Here we show several explicit examples of the differential formula.

- For $w \in \mathbb{Q} \langle e_0, e_1 \rangle$ whose last letter is not e_1 , we have

$$\begin{cases} \frac{d}{dz} L(e_z e_0 w) = -\frac{1}{z} L(e_z w), \\ \frac{d}{dz} L(e_z e_1 w) = -\frac{1}{z-1} L(e_z w) + \left(\frac{1}{z-1} - \frac{1}{z} \right) L(e_1 w). \end{cases} \quad (2.9)$$

- For $w \in \mathbb{Q} \langle e_0, e_z \rangle$, we have

$$\begin{cases} \frac{d}{dz} L(e_z w e_0) = -\frac{1}{z} L(e_z w), \\ \frac{d}{dz} L(e_1 e_z w e_0) = -\frac{1}{z} L(e_1 e_z w) + \frac{1}{z} L(e_1 w e_0) \\ \quad + \frac{1}{z-1} L((e_z - e_1) w e_0) \\ \frac{d}{dz} L(e_1 e_0 w e_0) = \frac{1}{z} L(e_1 w e_0) - \frac{1}{z} L(e_1 e_0 w). \end{cases} \quad (2.10)$$

3. PROOF OF MAIN THEOREM

3.1. Proof of Theorem 1.1. This subsection is devoted to giving a proof of the duality formula (Theorem 1.1). The result will be used to prove Theorem 1.2 in next subsection.

Proof of Theorem 1.1. Let τ be the anti-automorphism on \mathcal{A} , which was introduced in Section 1, defined as

$$\tau(e_0) = e_z - e_1, \quad \tau(e_1) = e_z - e_0, \quad \tau(e_z) = e_z.$$

Note that τ can be restricted to an anti-automorphism on the subset \mathcal{A}^0 of convergent words. Let γ be the Möbius transformation

$$\gamma(t) = \frac{zt - z}{t - z}$$

which acts on \mathbb{P}^1 and induces a permutation of $\{0, 1, z, \infty\}$ as

$$\gamma(0) = 1, \quad \gamma(1) = 0, \quad \gamma(\infty) = z, \quad \gamma(z) = \infty.$$

The Möbius transform γ induces a linear transformation on the holomorphic 1-forms $\omega_a(t) = dt/(t - a)$ ($a \in \{0, 1, z\}$) on $\mathbb{P}^1 - \{0, 1, z, \infty\}$ of the forms

$$\omega_0(t) = \omega_1(t') - \omega_z(t'), \quad \omega_1(t) = \omega_0(t') - \omega_z(t'), \quad \omega_z(t) = -\omega_z(t') \quad (t' = \gamma(t)).$$

For arbitrary real number z satisfying $z > 1$, we can verify that γ maps the segment $[0, 1] \subset \mathbb{P}^1$ to itself with opposite orientation. Thus, we obtain the desired formula

$$L(w - \tau(w)) = 0 \quad (w \in \mathcal{A}^0) \quad (3.1)$$

for such values of z . After the analytic continuation, we can conclude that the equality (3.1) holds for any $z \in \mathbb{C} \setminus [0, 1]$ by the identity theorem. This completes the proof of Theorem 1.1. \square

Remark 3.1.

- For any convergent word $w \in \mathcal{A}^0$, we know that

$$\lim_{z \rightarrow \infty} L(w) = L(w|_{e_z=0}) \quad (3.2)$$

holds. In particular, for any $w \in \mathbb{Q}\langle e_0, e_1 \rangle \cap \mathcal{A}^0$, the limit $z \rightarrow \infty$ of our duality formula (3.1) is reduced to

$$\lim_{z \rightarrow \infty} L(w - \tau(w)) = L(w - \tau_\infty(w)) = 0, \quad (3.3)$$

where τ_∞ is anti-endomorphism on \mathcal{A}^0 defined by

$$\tau_\infty(e_0) = -e_1, \quad \tau_\infty(e_1) = -e_0, \quad \tau_\infty(e_z) = 0.$$

The equality (3.3) is nothing but the duality formula (1.3) for multiple zeta values (see [9] and [16]).

- Evaluating (3.1) at $z = -1$, we also have

$$L(w - \tau(w)) \big|_{z=-1} = 0 \quad (w \in \mathcal{A}^0).$$

This relation is called the Broadhurst duality formula [1] (see also [13]).

Example 3.2. Substituting $w = e_z^n e_0 e_z^m$ ($n \geq 1, m \geq 0$) into the theorem gives the following three term relation:

$$I(0; \{z\}^n, 0, \{z\}^m; 1) + I(0; \{z\}^m, 1, \{z\}^n; 1) - I(0; \{z\}^{n+m+1}; 1) = 0.$$

3.2. Proof of Theorem 1.2. In this subsection we prove Theorem 1.2 (the sum formula).

Proof of Theorem 1.2. For integers $k \geq 2$ and $r \geq 1$ satisfying $k \geq r$, put

$$\begin{aligned} f_{k,r}(z) &= \sum_{\substack{k_1 + \dots + k_r = k \\ k_i \geq 1, \ k_r \geq 2}} L(e_z e_0^{k_1-1} e_1 e_0^{k_2-1} \dots e_1 e_0^{k_r-1}) \\ g_{k,r}(z) &= L((e_1 - e_z)(e_0 - e_z)^{r-1} e_0^{k-r}) \\ h_{k,r} &= \sum_{\substack{k_1 + \dots + k_r = k \\ k_i \geq 1, \ k_r \geq 2}} L(e_1 e_0^{k_1-1} e_1 e_0^{k_2-1} \dots e_1 e_0^{k_r-1}) = \lim_{z \rightarrow 1+0} f_{k,r}(z). \end{aligned}$$

Theorem 1.2 is equivalent to

$$(-1)^r f_{k,r}(z) = -L(e_1 e_0^{k-1}) + g_{k,r}(z). \quad (3.4)$$

We prove Theorem 1.2 by induction on k . The case $k = 2$ is obvious from the definition. Fix $k \geq 3$ and assume that

$$(-1)^{r'} f_{k-1,r'}(z) = -L(e_1 e_0^{k-2}) + g_{k-1,r'}(z) \quad (1 \leq r' \leq k-1) \quad (3.5)$$

hold. Our goal is to prove (3.4) for any r satisfying $1 \leq r \leq k$ under this induction hypothesis.

The equality (3.4) for the case $r = 1$ follows from the definition. The case $r = k$ follows from the duality formulas (3.1) and (3.3) proved in the previous subsection as

follows:

$$\begin{aligned} L((e_1 - e_z)(e_0 - e_z)^{k-1}) &= (-1)^k L(\tau(e_1^{k-1}e_0)) \\ &= (-1)^k L(e_1^{k-1}e_0) \\ &= L(\tau_\infty(e_1e_0^{k-1})) = L(e_1e_0^{k-1}). \end{aligned}$$

Thus, to complete our induction, it is enough to prove (3.4) for the case $1 < r < k$. In that situation, the differential formula (2.2) shows the following.

Lemma 3.3. *For integers k, r satisfying $1 < r < k$, the following equalities hold.*

$$\frac{d}{dz}f_{k,r}(z) = -\frac{1}{z}f_{k-1,r}(z) - \frac{1}{z-1}f_{k-1,r-1}(z) + \left(\frac{1}{z-1} - \frac{1}{z}\right)h_{k-1,r-1}, \quad (3.6)$$

$$\frac{d}{dz}g_{k,r}(z) = -\frac{1}{z}g_{k-1,r}(z) + \frac{1}{z-1}g_{k-1,r-1}(z). \quad (3.7)$$

Proof of Lemma 3.3. The equality (3.6) can be easily derived from (2.9). Since

$$g_{k,r}(z) = L(e_1e_0(e_0 - e_z)^{r-2}e_0^{k-r}) - L(e_1e_z(e_0 - e_z)^{r-2}e_0^{k-r}) - L(e_z(e_0 - e_z)^{r-1}e_0^{k-r}),$$

the equality (2.10) implies (3.7). \square

Let us take the limit $z \rightarrow 1 + 0$ in (3.5). Since $\lim_{z \rightarrow 1+0} g_{k,r}(z) = 0$, we have

$$(-1)^{r-1}h_{k-1,r-1} = -L(e_1e_0^{k-2}). \quad (3.8)$$

This also shows that $(-1)^r h_{k,r}$ is in fact independent of r . From (3.6), (3.7), (3.8), and the induction hypothesis, we have

$$\frac{d}{dz}((-1)^r f_{k,r}(z) - g_{k,r}(z)) = 0.$$

This implies that $(-1)^r f_{k,r}(z) - g_{k,r}(z)$ is independent of z . Since we have

$$\lim_{z \rightarrow \infty} f_{k,r}(z) = 0, \quad \lim_{z \rightarrow \infty} g_{k,r}(z) = L(e_1e_0^{k-1})$$

by (3.2), we can conclude that (3.4) holds. Thus, Theorem 1.2 is proved. \square

Finally, we remark that the sum formula (1.5) for multiple zeta values ([6, 16]) is obtained from (3.4) after taking the limit $z \rightarrow 1 + 0$.

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