A GENERATING FUNCTION
FOR SUMS OF MULTIPLE ZETA VALUES
AND ITS APPLICATIONS

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Abstract. A generating function for specified sums of multiple zeta values is defined and a differential equation that characterizes this function is given. As applications, some relations for multiple zeta values over the field of rational numbers are discussed.

1. Introduction

There are two types of definitions for multiple zeta values ([1], [6]). For a multi-index \( k = (k_1, k_2, \ldots, k_n) \) \((k_i \in \mathbb{N}(i = 1, 2, \ldots, n), k_1 > 1)\), we set

\[
\zeta(k) = \sum_{m_1 > m_2 > \ldots > m_n > 0} \frac{1}{m_1^{k_1} m_2^{k_2} \ldots m_n^{k_n}}
\]

and

\[
\zeta^*(k) = \sum_{m_1 \geq m_2 \geq \ldots \geq m_n \geq 1} \frac{1}{m_1^{k_1} m_2^{k_2} \ldots m_n^{k_n}}.
\]

The former is normally called a multiple zeta value (MZV for short) and used mainly in the mathematical literatures ([10], [12], [13], [16], [17], etc.). In this article, we are concerned with the latter, which we call a multiple zeta-star value (MZSV for short) to distinguish them from MZVs. Let us remark, however, that the word “multiple zeta values” is sometimes used not only for MZVs but also for MZSVs, for there are \(\mathbb{Q}\)-linear relations between MZVs and MZSVs, and hence the \(\mathbb{Q}\)-algebras generated respectively by MZVs and by MZSVs are the same. As is shown in [1] and [15], some part of \(\mathbb{Q}\)-linear relations that hold among multiple zeta values can be described clearly by using MZSVs. In this article, we introduce a generating function of specified sums of MZSVs and give an ordinary differential equation that characterizes this function. Computing the value of the generating function for unit argument gives some information concerning the relations between MZSVs over \(\mathbb{Q}\). This analysis had been done for MZVs in [16]. Our aim is to give an MZSV version of [16]. As a matter of fact, [1] is a part of the answer to this
problem. To give the complete answer is not an easy task because we have to get special values of generalized hypergeometric series for the unit argument. In the second half of this article, we will present some partial answers which are obtained under specializations of parameters.

2. A Generating Function

For a multi-index \( \mathbf{k} = (k_1, k_2, \ldots, k_n) \) \((k_i \in \mathbb{N})\), we set

\[
\text{wt}(\mathbf{k}) = k_1 + k_2 + \cdots + k_n, \quad \text{dep}(\mathbf{k}) = n, \quad \text{ht}(\mathbf{k}) = \# \{ i \mid k_i > 1 \}
\]

and call them the weight, the depth, and the height of \( \mathbf{k} \), respectively. The multi-index \( \mathbf{k} \) is said to be admissible if \( k_1 > 1 \). Let \( k, n \) and \( s \) be nonnegative integers and let \( I(k, n, s) \) denote the set of all multi-indices of weight \( k \), depth \( n \) and of height \( s \). We denote by \( I_0(k, n, s) \) the set of all admissible multi-indices in \( I(k, n, s) \). Let \( X_0(k, n, s; t) \) denote the sum

\[
(2.1) \quad X_0(k, n, s; t) = \sum_{\mathbf{k} \in I_0(k, n, s)} L^*_k(t),
\]

where we set

\[
(2.2) \quad L^*_k(t) = L^*_{k_1,\ldots,k_n}(t) = \sum_{m_1 \geq m_2 \geq \cdots \geq m_n \geq 1} \frac{t^{m_1}}{m_1^{k_1}m_2^{k_2} \cdots m_n^{k_n}}.
\]

The right-hand side of (2.2) converges locally uniformly in the unit disk \(|t| < 1\) of the complex \( t \)-plane for every multi-index \( \mathbf{k} \). If \( \mathbf{k} \) is admissible, then the right-hand side also converges for \( t = 1 \) and the value of it coincides with \( \zeta^*(\mathbf{k}) \). Now we define a generating function \( \Phi^*_0(t) \) for MZSVs by

\[
(2.3) \quad \Phi^*_0(t) = \Phi^*_0(x, y, z; t) = \sum_{k, n, s} X_0(k, n, s; t)x^{k-n-s}y^{n-s}z^{2s-2}.
\]

**Theorem 2.1.** The formal power series \( \Phi^*_0(t) \) is a unique power series solution vanishing at \( t = 0 \) of the differential equation

\[
(2.4) \quad t^2(1-t) \frac{d^2w}{dt^2} + t \{(1-t)(1-x) - y\} \frac{dw}{dt} + (xy - z^2)w = t.
\]

Hence it converges locally uniformly and defines a holomorphic function in \(|t| < 1\).

**Proof.** We define another auxiliary formal power series \( \Phi^*(t) \) by

\[
(2.5) \quad \Phi^*(t) = \Phi^*(x, y, z; t) = \sum_{k, n, s} X(k, n, s; t)x^{k-n-s}y^{n-s}z^{2s},
\]

where we set

\[
(2.6) \quad X(k, n, s; t) = \sum_{\mathbf{k} \in I(k, n, s)} L^*_k(t).
\]

Using the formulas

\[
\frac{d}{dt} L^*_{k_1,\ldots,k_n}(t) = \begin{cases} \frac{1}{t} L^*_{k_1-1,k_2,\ldots,k_n}(t) & \text{if } k_1 \geq 2, \\ \frac{1}{t(1-t)} L^*_{k_2,k_3,\ldots,k_n}(t) & \text{if } k_1 = 1, n > 1 \end{cases}
\]
and
\[
\frac{d}{dt} L_1^*(t) = \frac{1}{1 - t}
\]
for the derivative of \( L_k^*(t) \), we obtain
\[
\frac{d}{dt} X_0(k, n, s; t) = \frac{1}{t} \left( X(k-1, n, s-1; t) - X_0(k-1, n, s-1; t) + X_0(k-1, n, s; t) \right),
\]
\[
\frac{d}{dt} \left( X(k, n, s; t) - X_0(k, n, s; t) \right) = \frac{1}{t(1 - t)} X(k - 1, n - 1, s; t).
\]
In terms of \( \Phi_0^*(t) \) and \( \Phi^*(t) \), we find
\[
\frac{d\Phi_0^*}{dt} = \frac{1}{y t} \left( \Phi^* - 1 - z^2 \Phi_0^* \right) + \frac{x}{t} \Phi_0^*, \quad \frac{d}{dt} \left( \Phi^* - z^2 \Phi_0^* \right) = \frac{y}{t(1 - t)} (\Phi^* - 1) + \frac{y}{1 - t}.
\]
Eliminating \( \Phi^* \), we see that \( w = \Phi_0^* \) satisfies (2.4). The homogeneous equation of (2.4) is an ordinary differential equation of Fuchsian type with regular singularities at \( t = 0, 1, \infty \), and the characteristic equation at \( t = 0 \) is \( \lambda^2 - (x + y)\lambda + xy - z^2 = 0 \). Hence the characteristic exponents at \( t = 0 \) are not positive integers for generic \( x, y, z \). Therefore (2.4) has a unique formal power series solution in \( t \) vanishing at \( t = 0 \) and it should converge locally uniformly in \( |t| < 1 \). This completes the proof. \( \square \)

Although (2.4) is obtained from \( \Phi_0^* \), it can be solved independently of its origin. We shall solve (2.4) in two different ways. First we set \( w = \sum_{n=1}^{\infty} a_n t^n \) and determine \( \{a_n\} \) so that \( w \) satisfies (2.4). Then we have a recurrence relation for \( \{a_n\} \):
\[
a_1 = \frac{1}{(1 - x)(1 - y) - z^2},
\]
\[
a_{n+1} = \frac{n(n - x)}{(n + 1 - x)(n + 1 - y) - z^2} a_n \quad (n = 1, 2, \ldots).
\]
Thus we obtain the following

**Proposition 2.2.** Let \( w \) denote a formal power series
\[
(2.7) \quad w = \sum_{n=1}^{\infty} a_n t^n
\]
with
\[
a_n = \frac{(n - 1)!(1 - x)(2 - x) \cdots (n - 1 - x)}{((1 - x)(1 - y) - z^2)((2 - x)(2 - y) - z^2) \cdots ((n - x)(n - y) - z^2)}.
\]
Then \( w \) is a solution to (2.4).

Next we employ the method of variation of constants. Let \( \alpha \) and \( \beta \) be the characteristic exponents at \( t = 0 \) of the homogeneous equation of (2.4):
\[
\alpha, \beta = \frac{x + y \pm \sqrt{(x - y)^2 + 4z^2}}{2}.
\]
We set
\[
\varphi_1(t) = t^\alpha F(\alpha, \alpha - x, \alpha - \beta + 1; t),
\]
\[
\varphi_2(t) = t^\beta F(\beta, \beta - x, \beta - \alpha + 1; t).
\]
Here $F(a, b, c; t)$ denotes the Gauss hypergeometric function. Then $(\varphi_1, \varphi_2)$ is a system of fundamental solutions of the homogeneous equation. By the standard method of solving inhomogeneous differential equation, we have

**Proposition 2.3.** Let $w$ denote a function

$$w(t) = u_1(t)\varphi_1(t) + u_2(t)\varphi_2(t),$$

where $u_1$ and $u_2$ satisfy

$$u_1'(t) = \frac{1}{\alpha - \beta} t^{-\alpha}(1-t)^{y-1}F(\beta, \beta - x, \beta - \alpha + 1; t),$$

$$u_2'(t) = \frac{1}{\beta - \alpha} t^{-\beta}(1-t)^{y-1}F(\alpha, \alpha - x, \alpha - \beta + 1; t).$$

Then $w$ is a solution to (2.4).

Hence if we choose the starting point of integration appropriately to get $u_1(t)$ and $u_2(t)$, we have the unique holomorphic solution at the origin in the form (2.8). For example, if $\text{Re} \alpha < 1$ and $\text{Re} \beta < 1$, we set

$$u_1(t) = \frac{1}{\alpha - \beta} \int_0^t s^{-\alpha}(1-s)^{y-1}F(\beta, \beta - x, \beta - \alpha + 1; s)ds,$$

$$u_2(t) = \frac{1}{\beta - \alpha} \int_0^t s^{-\beta}(1-s)^{y-1}F(\alpha, \alpha - x, \alpha - \beta + 1; s)ds.$$

Then we have the holomorphic solution $w$ in the form (2.8). In the sequel, we assume $\text{Re} \alpha < 1$ and $\text{Re} \beta < 1$ for the sake of simplicity.

### 3. Evaluation of the generating function for unit argument

By the definition of $\Phi_0^*$, the coefficient of $x^{k-n-s}y^{n-s}z^{2s-2}$ of its value $\Phi_0^*(1)$ at $t = 1$ is the sum of MZSVs with fixed weight $k$, depth $n$ and height $s$. By using Propositions 2.2, 2.3 and (2.9), (2.10), we may write it in two ways:

$$\Phi_0^*(1) = \sum_{n=1}^{\infty} a_n$$

and

$$\Phi_0^*(1) = u_1(1)\varphi_1(1) + u_2(1)\varphi_2(1).$$

Here $u_1(1), u_2(1)$ are given by

$$u_1(1) = \frac{1}{\alpha - \beta} \int_0^1 s^{-\alpha}(1-s)^{y-1}F(\beta, \beta - x, \beta - \alpha + 1; s)ds,$$

$$u_2(1) = \frac{1}{\beta - \alpha} \int_0^1 s^{-\beta}(1-s)^{y-1}F(\alpha, \alpha - x, \alpha - \beta + 1; s)ds$$

and $\varphi_1(1), \varphi_2(1)$ are evaluated by the Gauss formula [5, p. 104, (46)]:

$$\varphi_1(1) = \frac{\Gamma(\alpha - \beta + 1)\Gamma(x - \alpha - \beta + 1)}{\Gamma(1 - \beta)\Gamma(x - \beta + 1)},$$

$$\varphi_2(1) = \frac{\Gamma(\beta - \alpha + 1)\Gamma(x - \alpha - \beta + 1)}{\Gamma(1 - \alpha)\Gamma(x - \alpha + 1)}.$$
Thus we see that $\Phi^*_0(1)$ has the value
\[
\int_0^1 ds \ s^{-\beta}(1-s)^{y-1} \left\{ \frac{\Gamma(\beta - \alpha)\Gamma(x - \alpha + 1)}{\Gamma(1 - \alpha)\Gamma(x + 1)} F(\alpha, \alpha - x, \alpha - \beta + 1; s) + \frac{\Gamma(\alpha - \beta)\Gamma(x - \alpha + 1)}{\Gamma(1 - \beta)\Gamma(x - \beta + 1)} s^{\beta - \alpha} F(\beta - x, \beta - \alpha + 1; s) \right\}.
\]
Using one of the connection formulas for the Gauss hypergeometric functions (e.g., [5, p. 108, (43)]), we rewrite this into the following form:
\[
\frac{1}{1-y} \int_0^1 s^{-\beta} F(1 - \beta, 1 - \beta + x, 2 - y; 1 - s) ds.
\]
Hence we have

**Proposition 3.1.** Under the notation as above, the following equality holds:

\[
\Phi^*_0(1) = \frac{1}{1-y} \int_0^1 (1-t)^{-\beta} F(1 - \beta, 1 - \beta + x, 2 - y; t) dt.
\]

**Remark 3.2.** Taking term-by-term integration in the right-hand side of (3.7), we can rewrite it in the form
\[
\frac{1}{(1 - y)(1 - \beta)} 3F_2(1 - \beta, 1 - \beta + x, 1; 2 - y, 2 - \beta; 1),
\]
where $3F_2(a, b, c; a', b'; t)$ denotes the generalized hypergeometric function [5, p.182]:
\[
3F_2(a, b, c; a', b'; t) = \frac{\Gamma(a')\Gamma(b')}{\Gamma(a)\Gamma(b)\Gamma(c)} \sum_{n=0}^{\infty} \frac{\Gamma(a + n)\Gamma(b + n)\Gamma(c + n)}{\Gamma(a' + n)\Gamma(b' + n)n!} t^n.
\]

4. **Specializations of parameters**

In some special cases, we can evaluate $\Phi^*_0(1)$ in terms of well known quantities.

4.1. **The case where $y = x$.** The case where $y = x$ in (3.1) is investigated in [1].

We can evaluate the sum $\sum_{n=1}^{\infty} (a_n |_{y=x})$ by using the Gauss formula:

\[
\sum_{n=1}^{\infty} (a_n |_{y=x}) = \frac{1}{z} \sum_{l=1}^{\infty} (-1)^l \left( \frac{1}{x + z - l} - \frac{1}{x - z - l} \right).
\]

Comparing the coefficient of $x^{k-2s}z^{2s-2}$ of $\Phi^*_0(1)|_{y=x}$ with that of the right-hand side of (4.1), we have

\[
\sum_{k \in I_0(k,s)} \zeta^*(k) = 2 \left( \begin{array}{c} k - 1 \\ 2s - 1 \end{array} \right) (1 - 2^{1-k}) \zeta(k),
\]

which is the main result of [1]. Here we set $I_0(k,*,s) = \bigcup_n I_0(k,n,s)$. Setting $x = 0$ in (4.1), we have the generating function for $\zeta^*(\{2\}_s) := \zeta^*(2,\ldots,2)$:

\[
\sum_{s=1}^{\infty} \zeta^*(\{2\}_s) z^{2s-2} = 2 \sum_{l=1}^{\infty} (-1)^l \frac{(-1)^l}{z^2 - l^2}.
\]

Taking the expansion of the right-hand side in $z$ [18, (2.2.1)], we have

\[
2 \sum_{s=1}^{\infty} (1 - 2^{1-2s}) \zeta(2s) z^{2s-2}.
\]
Thus we have the explicit form of $\zeta^*\{\{2\}_s\}$:
\begin{equation}
\zeta^*\{\{2\}_s\} = 2(1 - 2^{1 - 2s})\zeta(2s),
\end{equation}
or equivalently,
\begin{equation}
\zeta^*\{\{2\}_s\} = (-1)^{s-1}2(2^{2s-1} - 1)\frac{B_{2s}}{(2s)!}\pi^{2s},
\end{equation}
where $B_m$ denote the Bernoulli numbers:
\[ \frac{te^t}{e^t - 1} = \sum_{m=0}^{\infty} B_m \frac{t^m}{m!}. \]

**Remark 4.1.** M. Kaneko has pointed out that (4.6) can also be obtained in an elementary way. That is, computing the expansion of
\begin{equation}
\frac{\pi z}{\sin \pi z} = \prod_{m=1}^{\infty} \left(1 - \frac{z^2}{m^2}\right)^{-1}
\end{equation}
yields (4.6). This function is clearly equal to the right-hand side of (4.3) up to some trivial factors. Note that
\begin{equation}
\frac{\sin \pi z}{\pi z} = \prod_{m=1}^{\infty} \left(1 - \frac{z^2}{m^2}\right)
\end{equation}
is a generating function for $\zeta(\{\{2\}_s\})$.

**4.2. The case where $z^2 = xy$.** Let us consider the case where $z^2 = xy$. Since $\alpha \beta = 0$, we may assume $\alpha = 0$ and hence $\beta = x + y$. It follows from (3.7) that
\[ \Phi^*_{\alpha}(1)|_{z^2=xy} = \frac{1}{1 - y} \int_{0}^{1} (1 - t)^{-x-y} F(1 - x - y, 1 - y, 2 - y; t) dt. \]
Replacing $F$ by its corresponding series expression and taking term-by-term integration yield
\[ \sum_{l=0}^{\infty} \frac{(1 - x - y)l}{l!(l + 1 - y)} \int_{0}^{1} (1 - t)^{-x-y} t^l dt = \frac{1}{x} \sum_{l=1}^{\infty} \left( \frac{1}{l - x - y} - \frac{1}{l - y} \right). \]
The Taylor expansion of the right-hand side with respect to $x, y$ can be computed easily:
\[ \frac{1}{x} \sum_{k,n} \frac{(k - 1)!}{(k - n)! (n - 1)!} \left( \sum_{l} \frac{1}{l^k} \right) x^{k-n} y^{n-1} = \sum_{k,n} \frac{(k - 1)}{(n - 1)} \zeta(k) x^{k-n-1} y^{n-1}. \]
Comparing the coefficient of $x^{k-n-1} y^{n-1}$ with that of $\Phi^*_{\alpha}(1)|_{z^2=xy}$, which is equal to $\sum_{k \in I_0(k, n)} \zeta^*(k)$, we have
\[ \sum_{k \in I_0(k, n, *)} \zeta^*(k) = \binom{k - 1}{n - 1} \zeta(k). \]
Here we set $I_0(k, n, *) = \bigcup_s I_0(k, n, s)$. Thus we have obtained a new proof of the sum formula for MZSVs ([11]). See [15] for another proof of it. We refer the reader to [8] for the equivalence of the sum formula of MZVs and that of MZSVs. See also [7], [20] for the proof of the sum formula for MZVs.
4.3. **The case where** $y = 0$. Next we set $y = 0$. This specialization gives the generating function of MZSVs with full height. The coefficients of the function are the collections of MZSVs $\zeta^*(k)$ for which every component of multi-index $k$ is greater than or equal to 2. We write

$$\Phi_0^*(x, z) = \Phi_0^*(1)|_{y=0} = \sum_{k,n} X_0(k, n; 1) x^{k-2n} z^{2n-2}$$

and evaluate it by using (3.7).

**Theorem 4.2.** The power series (4.9) is given by

$$\Phi_0^*(x, z) = -\frac{1}{z^2} \left( 1 - \exp \left( \sum_{n=2}^{\infty} \frac{\zeta(n)}{n} S_n(x, z) \right) \right),$$

where the polynomials $S_n(x, z) \in \mathbb{Z}[x, z]$ are defined by the formula

$$S_n(x, z) = \alpha^n + \beta^n - x^n,$$

where $\alpha, \beta = \frac{x \pm \sqrt{x^2 + 4z^2}}{2}$

or alternatively by the identity

$$\log \left( 1 + \frac{z^2}{1 - x - z^2} \right) = \sum_{n=1}^{\infty} \frac{S_n(x, z)}{n}$$

together with the requirement that $S_n(x, z)$ is a homogeneous polynomial of degree $n$. In particular, all of the coefficients $X_0(k, n; 1)$ of $\Phi_0^*(x, z)$ can be expressed as polynomials in $\zeta(2), \zeta(3), \ldots$ with rational coefficients.

**Proof.** Since $\alpha + \beta = x$ and $\alpha \beta = -z^2$, it follows from (3.7) that

$$\Phi_0^*(x, z) = \int_0^1 (1 - t)^{-\beta} F(1 - \beta, 1 + \alpha; 2; t) dt$$

holds. Term-by-term integration in the right-hand side and the Gauss formula yield

$$\Phi_0^*(x, z) = \sum_{k=0}^{\infty} \frac{(1-\beta)_k (1+\alpha)_k}{(k+1)! k!} \int_0^1 (1 - t)^{-\beta} t^k dt$$

$$= \sum_{k=0}^{\infty} \frac{(1+\alpha)_k}{(k+1)! (1-\beta+k)}$$

$$= \frac{1}{\alpha \beta} \left( 1 - \frac{\Gamma(1-\alpha) \Gamma(1-\beta)}{\Gamma(1-\alpha-\beta)} \right).$$

Combining this with the expansion

$$\Gamma(1 - x) = \exp \left( \gamma x + \sum_{n=2}^{\infty} \frac{\zeta(n)}{n} x^n \right),$$

we obtain (4.10).
4.4. The case where \( z = 0 \). Finally we consider the case where \( z = 0 \). We use (3.1) to evaluate \( \Phi_0^*(1)\big|_{z=0} \). Since we have, by a partial fraction decomposition,

\[
a_n\big|_{z=0} = \frac{(n-1)!}{(n-x)(1-y)(2-y)\cdots(n-y)} = \sum_{m=1}^{n} \frac{(-1)^{m-1}(n-1)!}{(m-1)!(n-m)! (n-x)(m-y)},
\]

we can compute the Taylor expansion of \( \sum a_n\big|_{z=0} \) in \( x, y \):

\[
\sum_{n=1}^{\infty} (a_n\big|_{z=0}) = \sum_{i,j=1}^{\infty} \sum_{n\geq m\geq 1} (-1)^{m-1} \frac{1}{n^i m^j} x^{i-1} y^{j-1}.
\]

Noting that

\[
\Phi_0^*(1)\big|_{z=0} = \sum_{k,n} X_0(k,n,1) x^{k-n-1} y^{n-1}
\]

and

\[
X_0(k,n,1) = \zeta^*(k-n+1,\{1\}_{n-1}) := \zeta^*(k-n+1,1,\ldots,1),
\]

we have the following expression:

**Proposition 4.3.** Let \( i \) and \( j \) be positive integers. Then

\[
\zeta^*(i+1,\{1\}_{j-1}) = \sum_{n\geq m\geq 1} (-1)^{m-1} \frac{1}{n^i m^j}.
\]

holds.

**Remark 4.4.** The left-hand side of (4.15) is \( \xi_j(i) \) of Arakawa-Kaneko [2] (see [1] also).

**Remark 4.5.** Comparing the definition of MZSVs with the right-hand side of (4.15), we observe that the following equality should hold for every fixed \( n \) and \( j \):

\[
\sum_{n\geq m_1\geq m_2\geq\cdots\geq m_{j-1}\geq 1} \frac{1}{m_1 m_2 \cdots m_{j-1}} = \sum_{m=1}^{n} (-1)^{m-1} \frac{1}{m^j}.
\]

This identity appears in Corollary 3 of [4].

**Remark 4.6.** A generating function for \( \zeta(m+2,\{1\}_n) \) is given in [3], [20]:

\[
\sum_{m,n\geq 1} x^{m+1} y^{n+1} \zeta(m+2,\{1\}_n) = 1 - \exp \left( \sum_{k\geq 2} \frac{x^k + y^k - (x+y)^k}{k} \zeta(k) \right).
\]

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