

Contents lists available at ScienceDirect

# Journal of Symbolic Computation

www.elsevier.com/locate/jsc



# A symbolic approach to multiple zeta values at negative integers



Lin Jiu<sup>a</sup>, Victor H. Moll<sup>b</sup>, Christophe Vignat<sup>b,c</sup>

- <sup>a</sup> Research Institute for Symbolic Computation, Johannes Kepler University, Linz, Austria
- <sup>b</sup> Department of Mathematics, Tulane University, New Orleans, USA
- <sup>c</sup> LSS/Supelec, Université Paris Sud Orsay, Paris, France

#### ARTICLE INFO

Article history: Received 25 October 2015 Accepted 1 December 2016 Available online 18 January 2017

Keywords: Multiple zeta value Analytic continuation Bernoulli symbol

#### ABSTRACT

A symbolic computation technique is used to derive closed-form expressions for an analytic continuation of the Euler–Zagier zeta function evaluated at negative integers. This continuation was recently proposed by Sadaoui. The approach presented here yields explicit contiguity identities, recurrences on the depth of the zeta values and their generating functions. Moreover, it allows to prove that the resulting multiple zeta values computed at negative integers coincide with those obtained by another analytic continuation technique that uses the Euler–MacLaurin summation formula.

© 2017 Elsevier Ltd. All rights reserved.

#### 1. Introduction

The multiple zeta functions, first introduced by Euler, generalized by Hoffman (1992) and Zagier (1994), appear in diverse areas such as quantum field theory (Broadhurst, 1986) and knot theory (Takamuki, 1999). These functions are defined as

$$\zeta_r(n_1, \dots, n_r) = \sum_{0 < k_1 < \dots < k_r} \frac{1}{k_1^{n_1} \cdots k_r^{n_r}},\tag{1}$$

where  $\{n_i\}$  are complex values, and (1) converges when the constraints

$$\sum_{i=1}^{k} \operatorname{Re}(n_{r+1-j}) > k, \quad 1 \le k \le r, \tag{2}$$

are satisfied (see Matsumoto, 2002, §3). The values at integer points  $\mathbf{n} = (n_1, \dots, n_r)$  satisfying (2) are called *multiple zeta values*. An equivalent definition of these values is

$$\zeta_r(n_1,\ldots,n_r) = \sum_{k_1=-\infty}^{\infty} \frac{1}{k_1^{n_1} (k_1 + k_2)^{n_2} \cdots (k_1 + \cdots + k_r)^{n_r}}.$$

The sum of the exponents  $n_1 + \cdots + n_r$  is called the *weight* of the zeta value, and the number r of these exponents is called its *depth*.

Zhao (2000) showed that the multiple zeta function has an analytic continuation to the whole space  $\mathbb{C}^r$ . Contrarily to the case of functions of a single complex variable, the uniqueness of analytic continuations for functions of several complex variables is not always ensured. This is known as the *Hartogs' phenomenon*. Details appear in Fuks (1963, §6) and Kytmanov and Myslivets (2015, Chpt. 3). This lack of uniqueness for the multiple zeta functions is also described in Zagier (1994, pp. 509). Several authors have recently proposed a variety of approaches to the analytic continuation problem. For instance, Akiyama et al. (2001) used the Euler–MacLaurin summation formula and Matsumoto (2003) the Mellin–Barnes integral formula.

Sadaoui (2014) used another analytic continuation technique – thereafter called Raabe's analytic continuation technique – based on *Raabe's identity* which links the multiple integral

$$Y_{\mathbf{a}}(\mathbf{n}) = \int_{[1,+\infty)^r} \frac{d\mathbf{x}}{(x_1 + a_1)^{n_1} (x_1 + a_1 + x_2 + a_2)^{n_2} \cdots (x_1 + a_1 + \cdots + x_r + a_r)^{n_r}}$$

to the multiple zeta function

$$Z(\mathbf{n}; \mathbf{z}) = \sum_{k_1 = 1}^{\infty} \frac{1}{(k_1 + z_1)^{n_1} (k_1 + z_1 + k_2 + z_2)^{n_2} \cdots (k_1 + z_1 + \cdots + k_r + z_r)^{n_r}}$$
(3)

by

$$Y_{\mathbf{0}}(\mathbf{n}) = \int_{[0,1]^r} Z(\mathbf{n}; \mathbf{z}) d\mathbf{z}.$$
 (4)

A classical inversion argument is then applied to obtain an analytic continuation of the multiple zeta function defined at negative integer arguments  $-\mathbf{n} = (-n_1, \dots, -n_r)$ . Section 7 presents the symbolic mechanism behind this argument in details. The argument is based on the following steps:

- 1. compute the integral  $Y_{\mathbf{a}}(\mathbf{n})$  for values of  $n_1, \ldots, n_r$  that satisfy the convergence conditions (2);
- 2. replace in the result the values  $\mathbf{n}$  by  $-\mathbf{n}$ : it is then shown that  $Y_{\mathbf{a}}(-\mathbf{n})$  is a polynomial in the variable  $\mathbf{a}$ :
- 3. replace in this polynomial the variables  $\mathbf{a} = (a_1, \dots, a_r)$  by  $(\mathcal{B}_1, \dots, \mathcal{B}_r)$ , where each Bernoulli symbol  $\mathcal{B}_k$  is forced to satisfy two evaluation rules:

**Evaluation rule** 1. each power  $\mathcal{B}_{k}^{p}$  of the Bernoulli symbol  $\mathcal{B}_{k}$  should be evaluated as

$$\mathcal{B}_{k}^{p} \to B_{p}$$
, the *p*-th Bernoulli number; (5)

**Evaluation rule** 2. for distinct symbols  $\mathcal{B}_1, \dots, \mathcal{B}_n$ , the product  $\mathcal{B}_1^{p_1} \cdots \mathcal{B}_n^{p_n}$  is evaluated as

$$\mathcal{B}_1^{p_1} \cdots \mathcal{B}_n^{p_n} \to B_{p_1} \cdots B_{p_n}. \tag{6}$$

In the exceptional case where the symbols  $\mathcal{B}_k$  and  $\mathcal{B}_l$  coincide, the first rule (5) produces

$$\mathcal{B}_1^{p_1} \cdots \mathcal{B}_n^{p_n} \to B_{p_1} \cdots B_{p_{\nu}+p_{\nu}} \cdots B_{p_n}. \tag{7}$$

**Example 1.** A multiple zeta value of depth 2 at negative integers, obtained by Sadaoui (2014) using Raabe's analytic continuation, is now evaluated using the rules above.

First evaluate  $Y_{a_1,a_2}(n_1,n_2)$  and replace  $(n_1,n_2)$  by  $(-n_1,-n_2)$  in the result to obtain

$$Y_{a_1,a_2}(-n_1,-n_2) = \frac{1}{n_2+1} \sum_{k_2=0}^{n_2+1} \sum_{l_1=0}^{n_2+1} \sum_{l_2=0}^{n_2+2-k_2} \sum_{l_2=0}^{k_2} \frac{\binom{n_2+1}{k_2} \binom{n_1+n_2+2-k_2}{l_1} \binom{k_2}{l_2}}{n_1+n_2+2-k_2} a_1^{l_1} a_2^{l_2}.$$

Then substitute the variables  $a_1$  and  $a_2$  with the Bernoulli symbols  $\mathcal{B}_1$  and  $\mathcal{B}_2$  to obtain

$$\zeta_{2}\left(-n_{1},-n_{2}\right)=\frac{1}{n_{2}+1}\sum_{k_{2}=0}^{n_{2}+1}\sum_{l_{1}=0}^{n_{2}+1}\sum_{l_{2}=0}^{k_{2}}\frac{\binom{n_{2}+1}{k_{2}}\binom{n_{1}+n_{2}+2-k_{2}}{l_{1}}\binom{k_{2}}{l_{2}}\binom{k_{2}}{l_{2}}}{n_{1}+n_{2}+2-k_{2}}\mathcal{B}_{1}^{l_{1}}\mathcal{B}_{2}^{l_{2}}.$$

Using the rules (5) and (6) for the Bernoulli symbols, the multiple zeta value of depth 2 at  $(-n_1, -n_2)$  is given by

$$\zeta_2\left(-n_1,-n_2\right) = \frac{1}{n_2+1} \sum_{k_2=0}^{n_2+1} \sum_{l_1=0}^{n_1+n_2+2-k_2} \sum_{l_2=0}^{k_2} \frac{\binom{n_2+1}{k_2} \binom{n_1+n_2+2-k_2}{l_1} \binom{k_2}{l_2}}{n_1+n_2+2-k_2} B_{l_1} B_{l_2}.$$

The general case (Sadaoui, 2014, eq. (4.10)) is presented by the (2r-1)-fold sum<sup>1</sup>

$$\zeta_{r}(-n_{1},...,-n_{r}) = \frac{(-1)^{r}}{n_{r}+1} \sum_{k_{2},...,k_{r}} \frac{1}{\left(\bar{n}+r-\bar{k}\right)} \prod_{j=2}^{r} \frac{\left(\sum_{i=j}^{r} n_{i}+r-j+1-\sum_{i=j+1}^{r} k_{i}\right)}{\left(\sum_{i=j}^{r} n_{i}+r-j+1-\sum_{i=j+1}^{r} k_{i}\right)} \times \sum_{l_{1},...,l_{r}} \left(\bar{n}+r-\bar{k}\right) \binom{k_{2}}{l_{2}} ... \binom{k_{r}}{l_{r}} B_{l_{1}} ... B_{l_{r}}, \tag{8}$$

where  $k_2, \ldots, k_r \ge 0$ ,  $l_j \le k_j$  for  $2 \le j \le r$  and  $l_1 \le \bar{n} + r + \bar{k}$  with

$$\bar{n} = \sum_{i=1}^{r} n_j, \ \bar{k} = \sum_{i=2}^{r} k_j.$$
 (9)

An alternative evaluation for (8) is proposed in this paper. This is used here to derive some specific zeta values at negative integers, contiguity identities for the multiple zeta functions, recursions on their depth and generating functions. This evaluation also allows us to prove that Sadaoui's analytic continuation based on Raabe's formula provides the exact same multiple zeta values at negative integers as the Euler–Maclaurin technique used in Akiyama and Tanigawa (2001).

#### 2. Main result

First, introduce the symbols  $C_{1,2,...,k}$ , defined recursively in terms of the Bernoulli symbols  $B_1, ..., B_r$  as

$$C_1^n = \frac{\mathcal{B}_1^n}{n}, \ C_{1,2}^n = \frac{(\mathcal{C}_1 + \mathcal{B}_2)^n}{n}, \dots, \ C_{1,2,\dots,k+1}^n = \frac{\left(\mathcal{C}_{1,2,\dots,k} + \mathcal{B}_{k+1}\right)^n}{n}. \tag{10}$$

Their symbolic computation rule is defined next.

<sup>&</sup>lt;sup>1</sup> This corrects a typo in Sadaoui (2014, eq. (1.6)).

C-symbols rule: Expand the symbols  $C_{1,2,...,k}$  using (10) to obtain expressions involving only Bernoulli symbols  $\mathcal{B}_k$ 's. These expressions are then simplified using the evaluation rules for Bernoulli symbols (5) and (6). The next example illustrates this procedure.

# Example 2. The term

$$C_1^{n_1}C_{1,2}^{n_2} = C_1^{n_1} \frac{(C_1 + B_2)^{n_2}}{n_2} = \sum_{k=0}^{n_2} \binom{n_2}{k} \frac{C_1^{n_1+k}B_2^{n_2-k}}{n_2} = \sum_{k=0}^{n_2} \binom{n_2}{k} \frac{B_1^{n_1+k}B_2^{n_2-k}}{(n_1+k)n_2}$$

is evaluated as

$$\frac{1}{n_2} \sum_{k=0}^{n_2} {n_2 \choose k} \frac{B_{n_1+k}}{n_1+k} B_{n_2-k}.$$

The main result now gives a symbolic evaluation of the multiple zeta value at negative integers.

**Theorem 3.** The multiple zeta value (8) at the negative integers  $(-n_1, \ldots, -n_r)$  produced by Raabe's analytic continuation is given by

$$\zeta_r(-n_1,\ldots,-n_r) = \prod_{k=1}^r (-1)^{n_k} C_{1,\ldots,k}^{n_k+1}.$$
(11)

**Proof.** The inner sum in (8), in its Bernoulli-symbols version,

$$\sum_{l_1,\ldots,l_r} {\bar{n}+r-\bar{k} \choose l_1} {k_2 \choose l_2} \cdots {k_r \choose l_r} \mathcal{B}_1^{l_1} \cdots \mathcal{B}_r^{l_r}$$

can be summed to

$$(1+\mathcal{B}_1)^{\bar{n}+r-\bar{k}}(1+\mathcal{B}_2)^{k_2}\cdots(1+\mathcal{B}_r)^{k_r}$$

The classical identity<sup>2</sup> for the Bernoulli symbol  $\mathcal{B}+1=-\mathcal{B}$ , with  $\bar{n}$  and  $\bar{k}$  defined in (9), reduces this to

$$(-1)^{\bar{n}+r} \mathcal{B}_1^{\bar{n}+r-\bar{k}} \mathcal{B}_2^{k_2} \cdots \mathcal{B}_r^{k_r}. \tag{12}$$

It follows that

$$\zeta_r(-\mathbf{n}) = \frac{(-1)^{\bar{n}}}{(n_r+1)} \sum_{k_2,\dots,k_r} C_1^{\bar{n}+r-\bar{k}} \mathcal{B}_2^{k_2} \cdots \mathcal{B}_r^{k_r} \prod_{j=2}^r \frac{\left(\sum\limits_{i=j}^r n_i + r - j + 1 - \sum\limits_{i=j+1}^r k_i\right)}{\left(\sum\limits_{i=j}^r n_i + r - j + 1 - \sum\limits_{i=j+1}^r k_i\right)}.$$

Summing first over  $k_2$  gives

$$\exp(z\mathcal{B}) = \frac{z}{\exp(z) - 1}.$$

<sup>&</sup>lt;sup>2</sup> This identity can be easily deduced from the generating function

$$\zeta_r(-\mathbf{n}) = \frac{(-1)^{\bar{n}}}{(n_r+1)} \sum_{k_3,\dots,k_r} C_1^{n_1+1} C_2^{n_2+\dots+n_r+r-1} \mathcal{B}_3^{k_3} \cdots \mathcal{B}_r^{k_r} \prod_{j=3}^r \frac{\left(\sum\limits_{i=j}^r n_i + r - j + 1 - \sum\limits_{i=j+1}^r k_i\right)}{\left(\sum\limits_{i=j}^r n_i + r - j + 1 - \sum\limits_{i=j+1}^r k_i\right)}.$$

Now sum over the remaining indices in order to obtain the result.  $\Box$ 

We remark that the reduction (12) performed in the proof gives a simpler version of Sadaoui's formula (8) as the more tractable (r-1)-fold sum

$$\zeta_{r}(-n_{1},\ldots,-n_{r}) = \frac{(-1)^{\bar{n}}}{n_{r}+1} \sum_{k_{2},\ldots,k_{r}} \frac{1}{\left(\bar{n}+r-\bar{k}\right)} \prod_{j=2}^{r} \frac{\left(\sum_{i=j}^{r} n_{i}+r-j+1-\sum_{i=j+1}^{r} k_{i}\right) B_{l_{1}} \cdots B_{l_{r}}}{\left(\sum_{i=j}^{r} n_{i}+r-j+1-\sum_{i=j+1}^{r} k_{i}\right)}.$$
 (13)

Moreover, the derivation of (11) is unchanged if each symbol  $\mathcal{B}_i$  is replaced by the *polynomial Bernoulli symbol*  $\mathcal{B}_i + z$  defined by

$$\left(\mathcal{B}_{i}+z\right)^{n}=B_{n}\left(z\right),$$

where  $B_n(z)$  is the Bernoulli polynomial of degree n. The same proof as above yields the next statement.

**Theorem 4.** Raabe's analytic continuation of the multiple zeta function  $\zeta_r(\mathbf{n}; \mathbf{z}) = Z(\mathbf{n}; \mathbf{z})$  defined by (3) can be written as

$$\zeta_r(-n_1,\ldots,-n_r;z_1,\ldots,z_r) = \prod_{k=1}^r (-1)^{n_k} C_{1,\ldots,k}^{n_k+1}(z_1,\ldots,z_k), \qquad (14)$$

with

$$C_1^n(z_1) = \frac{(z_1 + \mathcal{B}_1)^n}{n} = \frac{B_n(z_1)}{n}, \ C_{1,2}^n(z_1, z_2) = \frac{(C_1(z_1) + \mathcal{B}_2 + z_2)^n}{n}, \dots$$

and

$$C_{1,2,\ldots,k+1}^n(z_1,\ldots,z_{k+1}) = \frac{\left(C_{1,2,\ldots,k}(z_1,\ldots,z_k) + \mathcal{B}_{k+1} + z_{k+1}\right)^n}{n}.$$

# 3. A general recursion formula on the depth

A recursion formula for the zeta function, based on depth, is produced next.

**Theorem 5.** The multiple zeta functions satisfy the recursion rule

$$\zeta_r(-\mathbf{n}; \mathbf{z}) = \frac{(-1)^{n_r}}{n_r + 1} \sum_{l=0}^{n_r + 1} {n_r + 1 \choose l} (-1)^l \zeta_{r-1}(-n_1, \dots, -n_{r-1} - l; \mathbf{z}) B_{n_r + 1 - l}(z_r).$$
 (15)

Introduce the new zeta symbol  $\mathcal{Z}_r$ , with the evaluation rule<sup>3</sup>

$$\mathcal{Z}_r^l = \zeta_r (-n_1, \dots, -n_{r-1}, -n_r - l; \mathbf{z});$$

<sup>&</sup>lt;sup>3</sup> Note that  $\mathcal{Z}_r^0 \neq 1$ .

then (15) can be written symbolically as

$$\zeta_r(-\mathbf{n}; \mathbf{z}) = (-1)^{n_r} \frac{(\mathcal{B} - \mathcal{Z}_{r-1})^{n_r+1}}{n_r + 1} = \zeta_1(-n_r; -\mathcal{Z}_{r-1}).$$
(16)

**Proof.** Expand the last term of (14)

$$C_{1,\dots,r}^{n_r+1}(z_1,\dots,z_r) = \frac{\left(C_{1,\dots,r-1}^{n_r-1+1}(z_1,\dots,z_{r-1}) + \mathcal{B}_r(z_r)\right)^{n_r+1}}{n_r+1}$$

using the binomial theorem to produce

$$\zeta_{r}(-\mathbf{n}; \mathbf{z}) = \frac{(-1)^{n_{r}}}{n_{r}+1} \sum_{l=0}^{n_{r}+1} {n_{r}+1 \choose l} \left( \prod_{k=1}^{r-1} (-1)^{n_{k}} C_{1,\dots,k}^{n_{k}+1}(z_{1},\dots,z_{k}) \right) \times C_{1}^{l} \qquad r-1 (z_{1},\dots,z_{r-1}) \mathcal{B}_{r}^{n_{r}+1-l}(z_{r}).$$

Then identify

$$\left(\prod_{k=1}^{r-1} (-1)^{n_k} \mathcal{C}_{1,\dots,k}^{n_k+1}(z_1,\dots,z_k)\right) \mathcal{C}_{1,\dots,r-1}^l(z_1,\dots,z_{r-1})$$

$$= (-1)^l \zeta_{r-1}(-n_1,\dots,-n_{r-2},-n_{r-1}-l;\mathbf{z}),$$

to obtain the desired result.

This identity can be written as

$$\zeta_r(-n_1,\ldots,-n_r;z_1,\ldots,z_r) = \frac{(-1)^{n_r}}{n_r+1} (\mathcal{B} - \mathcal{Z}_{r-1})^{n_r+1}$$

with the initial value

$$\zeta_1(-n;z) = (-1)^n \frac{(z+B)^{n+1}}{n+1}.$$

#### 4. Contiguity identities

Raabe's analytic continuation of the multiple zeta functions at negative integers satisfies contiguity identities in the **z** variables. Two of them are presented here.

**Theorem 6.** The multiple zeta functions satisfy:

$$\zeta_r (-n_1, \dots, -n_r; z_1, \dots, z_{r-1}, z_r + 1)$$

$$= \zeta_r (-n_1, \dots, -n_r; z_1, \dots, z_{r-1}, z_r) + (-1)^{n_r} (z_r - \mathcal{Z}_{r-1})^{n_r}.$$

**Example 7.** Theorem 6, in the case of depth 2, gives

$$\zeta_2(-n_1, -n_2, z_1, z_2 + 1) = \zeta_2(-n_1, -n_2, z_1, z_2) + (-1)^{n_1+1} (z_2 - \mathcal{Z}_1)^{n_2}.$$

The second term is now expanded as

$$(-1)^{n_1+1} \sum_{l=0}^{n_2} {n_2 \choose l} z_2^{n_2-l} (-1)^l \zeta_1 (-n_1-l; z_1),$$

to produce the contiguity identity.

**Proof of Theorem 6.** Expand

$$\zeta_{r}(-n_{1},\ldots,-n_{r};z_{1},\ldots,z_{r-1},z_{r}+1) \\
= \frac{(-1)^{\bar{n}}}{n_{r}+1} \prod_{k=1}^{r-2} \mathcal{C}_{1,\ldots,k}^{n_{k}+1}(z_{1},\ldots,z_{k}) \sum_{l=0}^{n_{r}+1} \binom{n_{r}+1}{l} (-1)^{l} \mathcal{C}_{1,\ldots,r-1}^{n_{r-1}+1+l}(z_{1},\ldots,z_{r-1}) B_{n_{r}+1-l}(z_{r}+1),$$

and use the identity for Bernoulli polynomials

$$B_{n_r+1-l}(z_r+1) = B_{n_r+1-l}(z_r) + (n_r-l+1)z_r^{n_r-l}$$

to produce the result.  $\Box$ 

The corresponding result for a shift in the first variable, stated next, admits a similar proof.

**Theorem 8.** The depth-2 multiple zeta function satisfies the contiguity identity

$$\zeta_2(-n_1,-n_2;z_1+1,z_2) = \zeta_2(-n_1,-n_2;z_1,z_2) + \frac{(-1)^{n_1+n_2}}{n_2+1}z_1^{n_1}B_{n_2+1}(z_1+z_2).$$

# 5. Generating function

A generating function for the multiple zeta values at negative integers is defined by

$$F_r(w_1, \dots, w_r) = \sum_{n_1, \dots, n_r > 0} \frac{w_1^{n_1} \cdots w_r^{n_r}}{n_1! \cdots n_r!} \zeta_r(-n_1, \dots, -n_r).$$
(17)

A recurrence for  $F_r$  is presented below. The initial condition is given in terms of the generating function for Bernoulli numbers

$$F_B(w) = \sum_{n=0}^{\infty} \frac{B_n}{n!} w^n = \frac{w}{e^w - 1}.$$

**Theorem 9.** The generating function (17) for the multiple zeta values at negative integers satisfies the recurrence

$$F_r(w_1, \dots, w_r) = \frac{1}{w_r} \Big( F_{r-1}(w_1, \dots, w_{r-1}) - F_B(-w_r) F_{r-1}(w_1, \dots, w_{r-2}, w_{r-1} + w_r) \Big),$$
(18)

with initial value

$$F_1(w_1) = -\frac{1}{w_1} \left( e^{-w_1 \mathcal{B}_1} - 1 \right) = \frac{1 - F_B(-w_1)}{w_1}.$$

Proof. Start from

$$F_r(w_1,\ldots,w_r) = \sum_{n_1,\ldots,n_r} \frac{w_1^{n_1}\cdots w_r^{n_r}}{n_1!\cdots n_r!} (-1)^{n_1+\cdots+n_r} C_1^{n_1+1}\cdots C_{1,\ldots,r}^{n_r+1} = \prod_{j=1}^r C_{1,\ldots,j} e^{-w_j C_{1,\ldots,j}},$$

and expand

$$C_{1,\dots,r}e^{-w_rC_{1,\dots,r}} = \sum_{n=0}^{\infty} \frac{(-w_r)^n}{n!} \cdot \frac{(-1)^{n+1}}{n+1} \left( C_{1,\dots,r-1} + \mathcal{B}_r \right)^{n+1} = -\frac{1}{w_r} \left( e^{-w_r(C_{1,\dots,r-1} + \mathcal{B}_r)} - 1 \right),$$

to deduce that

$$\begin{split} &F_{r}\left(w_{1},\ldots,w_{r}\right)\\ &=\frac{1}{w_{r}}\left(\prod_{j=1}^{r-1}\mathcal{C}_{1,\ldots,j}e^{-w_{j}\mathcal{C}_{1,\ldots,j}}\right)-\frac{1}{w_{r}}\left(\prod_{j=1}^{r-2}\mathcal{C}_{1,\ldots,j}e^{-w_{j}\mathcal{C}_{1,\ldots,j}}\right)e^{-w_{r}\mathcal{B}_{r}}\mathcal{C}_{1,\ldots,r-1}e^{-\left(w_{r-1}+w_{r}\right)\mathcal{C}_{1,\ldots,r-1}}\\ &=\frac{1}{w_{r}}F_{r-1}\left(w_{1},\ldots,w_{r-1}\right)-\frac{1}{w_{r}}F_{B}\left(-w_{r}\right)F_{r-1}\left(w_{1},\ldots,w_{r-2},w_{r-1}+w_{r}\right). \end{split}$$

This completes the argument.  $\Box$ 

Remark 10. Using the shift operator

$$f(w+a) = \exp\left(a\frac{\partial}{\partial w}\right) \circ f(w)$$

and  $F_1(w, z) = -\frac{1}{w} \left( e^{-w(\mathcal{B}+z)} - 1 \right)$  gives the recurrence (18) in the form

$$F_r(w_1,...,w_r) = F_1\left(w_r, -\frac{\partial}{\partial w_{r-1}}\right) \circ F_{r-1}(w_1,...,w_{r-1}).$$

It follows that the generating function can be symbolically expressed as the r-fold composition

$$F_r(w_1, \dots, w_r) = F_1\left(w_r, -\frac{\partial}{\partial w_{r-1}}\right) \circ F_1\left(w_{r-1}, -\frac{\partial}{\partial w_{r-2}}\right) \circ \dots \circ F_1\left(w_2, -\frac{\partial}{\partial w_1}\right)$$

$$\circ F_1(w_1).$$

# 6. Quasi-shuffle identity

Multiple zeta values at positive integers satisfy quasi-shuffle identities, exemplified by

$$\zeta_2(n_1, n_2) + \zeta_2(n_2, n_1) + \zeta_1(n_1 + n_2) = \zeta_1(n_1)\zeta_1(n_2).$$
 (19)

Some analytic continuations, such as the one given in (Manchon and Paycha, 2010), preserve this relation, while Raabe's analytic continuation used in (Sadaoui, 2014) does not. The next theorem gives the correction term.

**Theorem 11.** The multiple zeta values at negative integers satisfy the identity

$$\zeta_{2}(-n_{1}, -n_{2}) + \zeta_{2}(-n_{2}, -n_{1}) + \zeta_{1}(-n_{1} - n_{2}) - \zeta_{1}(-n_{1})\zeta_{1}(-n_{2}) 
= \frac{(-1)^{n_{1}+1}n_{1}!n_{2}!}{(n_{1}+n_{2}+2)!}B_{n_{1}+n_{2}+2}.$$
(20)

**Remark 12.** When  $n_1 + n_2$  is odd, the Bernoulli number  $B_{n_1 + n_2 + 2} = 0$  so that the quasi-shuffle identity (19) holds for  $\zeta_2(-n_1, -n_2)$  as expected, since the depth-2 multiple zeta function is holomorphic at these points.

### **Proof of Theorem 11.** Let

$$\delta(w_1, w_2) = F_2(w_1, w_2) + F_2(w_2, w_1) + F_1(w_1 + w_2) - F_1(w_1) F_1(w_2)$$

with  $F_1$  and  $F_2$  defined in (17). An elementary calculation gives

$$\delta(w_1, w_2) = \frac{\frac{1}{w_1} + \frac{1}{w_2} - \frac{1}{2}\coth\left(\frac{w_1}{2}\right) - \frac{1}{2}\coth\left(\frac{w_2}{2}\right)}{w_1 + w_2}.$$

The expansions

$$\frac{1}{w_1} - \frac{1}{2} \coth\left(\frac{w_1}{2}\right) = -\sum_{k=0}^{\infty} \frac{w_1^{2k+1}}{(2k+2)!} B_{2k+2} \text{ and } \frac{1}{w_1 + w_2} = \frac{1}{w_2} \sum_{k>0} \left(-\frac{w_1}{w_2}\right)^{\ell}$$

now produce

$$\delta\left(w_{1},w_{2}\right)=-\sum_{k,l=0}^{\infty}\left(-1\right)^{l}\frac{B_{2k+2}}{(2k+2)!}\left(w_{1}^{2k+l+1}w_{2}^{-l-1}+w_{1}^{l}w_{2}^{2k-l}\right).$$

Identifying the coefficient of  $w_1^{n_1}w_2^{n_2}$  in this series expansion gives the result.  $\Box$ 

# 7. A symbolic derivation of Raabe's identity and its associated analytic continuation technique

The symbolic method developed here is now used to explain the mechanism behind this classical identity. In order to achieve this, define the uniform symbol  $\mathcal{U}$  on [0,1] by its generating function

$$\exp\left(z\mathcal{U}\right) = \frac{e^z - 1}{z}.$$

Observe that, since  $\exp(z\mathcal{B}) = \frac{z}{\exp(z)-1}$ ,

$$\exp(z\mathcal{B})\exp(z\mathcal{U}) = \exp(z(\mathcal{B} + \mathcal{U})) = 1,$$

so that for any analytic function f whose Taylor expansion converges uniformly on  $\mathbb{R}$ ,

$$f(z + U + B) = f(z)$$
.

Define the new symbol  $\mathcal V$  by

$$f(z+V) = \int_{1}^{\infty} f(z+v) dv,$$

and observe that

$$f(z+V) = \sum_{k\geq 1} \int_{k}^{k+1} f(z+v) \, dv = \sum_{k\geq 1} \int_{0}^{1} f(z+v+k) \, dv = \sum_{k\geq 1} f(z+k+U)$$

so that, by replacing z by  $z + \mathcal{B}$ ,

$$f(z+\mathcal{V}+\mathcal{B}) = \sum_{k\geq 1} f(z+k).$$

Repeating this operation gives the symbolic expression of Raabe's identity for r = 2:

$$\sum_{k_1, k_2 \ge 1} f_1(z_1 + k_1) f_2(z_1 + k_1 + x_2 + k_2)$$
  
=  $f_1(z_1 + \mathcal{V}_1 + \mathcal{B}_1) f_2(z_1 + \mathcal{V}_1 + \mathcal{B}_1 + z_2 + \mathcal{V}_2 + \mathcal{B}_2)$ .

Extending this to an arbitrary value of r gives Raabe's formula (4). The details are left to the reader.

**Example 13.** The case r = 1 provides the simplest version of the formalism introduced here. The Hurwitz zeta function is

$$\zeta(z;n) = \sum_{k=1}^{\infty} \frac{1}{(z+k)^n}.$$

Now

$$\zeta(z+U;n) = \sum_{k=1}^{\infty} \frac{1}{(z+U+k)^n} = \frac{1}{n-1} (z+1)^{1-n}$$

so that formally,

$$\zeta(z; n) = \zeta(z + \mathcal{U} + \mathcal{B}; n) = \frac{1}{n-1}(z + \mathcal{B} + 1)^{1-n}.$$

Replacing n by -2n gives

$$\zeta(z; -2n) = \frac{-1}{2n+1} B_{2n+1}(z+1).$$

This is the well-known formula for the analytic continuation of the Hurwitz zeta function and illustrate the mechanism behind Raabe's identity.

# 8. Specific multiple zeta values

This section gives some examples of the evaluation at negative integers.

# Example 14.

1) For depth r = 2,

$$\zeta_2(-n,0) = (-1)^n \left( \frac{B_{n+2}}{n+2} - \frac{1}{2} \frac{B_{n+1}}{n+1} \right),$$

and

$$\zeta_2(0,-n) = \frac{(-1)^{n+1}}{n+1} (B_{n+1} + B_{n+2}).$$

2) For depth r = 3,

$$\zeta_3(-n,0,0) = \frac{(-1)^n}{2} \left( \frac{B_{n+3}}{n+3} - 2 \frac{B_{n+2}}{n+2} + \frac{2}{3} \frac{B_{n+1}}{n+1} \right)$$

and

$$\zeta_3(0, -n, 0) = \frac{(-1)^{n+1}}{2} \left( \frac{n}{(n+1)(n+2)} B_{n+2} - \frac{B_{n+1}}{n+1} + 2 \frac{B_{n+3}}{n+2} \right).$$

3) As a final example, the recursion rule (15) is used to compute the value  $\zeta_3$  (0, 0, -2):

$$\zeta_{3}(0,0,-2) = \frac{(\mathcal{B} - \mathcal{Z}_{2})^{3}}{3} 
= \frac{1}{3} \left( \mathcal{B}^{3} \mathcal{Z}_{2}^{0} - 3\mathcal{B}^{2} \mathcal{Z}_{2}^{1} + 3\mathcal{B} \mathcal{Z}_{2}^{2} - \mathcal{Z}_{2}^{3} \right) 
= \frac{1}{3} (B_{3} \zeta_{2}(0,0) - 3B_{2} \zeta_{2}(0,-1) + 3B_{1} \zeta_{2}(0,-2) - \zeta_{2}(0,-3)) 
= -\frac{1}{60}.$$

A table of examples of  $\zeta$  (-a, -b) for  $0 \le a$ ,  $b \le 5$  is given in Sadaoui (2014, pp. 983). Comparable tables, produced by different analytic continuation techniques, are offered by Ebrahimi-Fard et al. (2002) and Guo and Zhang (2008).

#### 9. Connection to Euler-Maclaurin summation method

As mentioned in the introduction, Akiyama and Tanigawa (2001) considered the method of Euler–Maclaurin summation to define an analytic continuation of multiple zeta values at non-positive integers. One of their main results is the following recurrence (the notation  $\bar{\zeta}$  instead of  $\zeta$  will be used throughout, to distinguish this Euler–Maclaurin analytic continuation from the Raabe analytic continuation described above):

$$\bar{\zeta}_{k}(-r_{1}, -r_{2}, \dots, -r_{k}) = -\frac{\bar{\zeta}_{k-1}(-r_{1}, -r_{2}, \dots, -r_{k-2}, -r_{k-1} - r_{k} - 1)}{r_{k} + 1} - \frac{\bar{\zeta}_{k-1}(-r_{1}, -r_{2}, \dots, -r_{k-2}, -r_{k-1} - r_{k})}{2} + \sum_{q=1}^{r_{k}} (-r_{k})_{q} a_{q} \bar{\zeta}_{k-1}(-r_{1}, -r_{2}, \dots, -r_{k-2}, -r_{k-1} - r_{k} + q), \quad (21)$$

where

$$(-r_k)_q = (-r_k)(-r_k+1)\cdots(-r_k+q-1) = \frac{\Gamma(-r_k+q)}{\Gamma(a)}$$

is the Pochhammer symbol and

$$a_q := \frac{B_{q+1}}{(q+1)!}.$$

The recurrence (21) yields the values for k = 2

-						
$\overline{\zeta}_2(-n,-m)$	m = 0	m = 1	m = 2	m = 3	m = 4	m = 5
n = 0	<u>1</u> 3	1/12	1 90	$-\frac{1}{120}$	$-\frac{1}{210}$	1 252
n = 1	$\frac{1}{24}$	1 360	$-\frac{1}{240}$	$-\frac{1}{560}$	<u>1</u> 504	1 504
n = 2	$-\frac{1}{120}$	$-\frac{1}{240}$	$-\frac{1}{15120}$	1 504	29 37800	$-\frac{1}{480}$
n = 3	$-\frac{1}{240}$	13 10080	1 504	1 50400	$-\frac{1}{480}$	$-\frac{557}{665280}$
n = 4	1 252	1 504	$-\frac{11}{15120}$	$-\frac{1}{480}$	$-\frac{1}{166320}$	1 264
n = 5	<u>1</u> 504	$-\frac{53}{30240}$	$-\frac{1}{480}$	109 133056	1 264	739 181621440

We remark that these values coincide with those provided by Rabbe's analytic continuation. Further study reveals that such agreement is true for arbitrary depth, as stated in the next theorem.

**Theorem 15.** For any  $k \in \mathbb{N}$ , the multiple zeta values at negative integers produced by the Euler–MacLaurin analytic continuation method satisfy

$$\bar{\zeta}_k(-r_1,\ldots,-r_k) = \prod_{j=1}^k (-1)^{r_j} C_{1,\ldots,j}^{r_j+1}.$$

Thus, by Theorem 3, they coincide with the values produced by Raabe's analytic continuation method.

**Proof.** Special values of Pochhammer symbol and Bernoulli numbers are

$$(-x)_{-1} = \frac{\Gamma(-x-1)}{\Gamma(-x)} = \frac{1}{-x-1} = -\frac{1}{x+1}, \ (-x)_0 = 1, \ \frac{B_0}{0!} = B_0 = 1, \ \frac{B_1}{1!} = -\frac{1}{2},$$

which, together with the identity

$$\frac{(-r_k)_{q-1}}{q!} = \frac{(-r_k)\cdots(-r_k+q-2)}{q!} = \frac{(-1)^{q-1}}{r_k+1} {r_k+1 \choose q},$$

allow to simplify the recurrence (21) to

$$\bar{\zeta}_{k}\left(-r_{1}, -r_{2}, \dots, -r_{k}\right) \\
= -\frac{1}{r_{k}+1} \sum_{q=0}^{r_{k}+1} {r_{k}+1 \choose q} \left(-\mathcal{B}_{k}\right)^{q} \bar{\zeta}_{k-1} \left(-r_{1}, \dots, -r_{k-2}, -r_{k-1} - r_{k} - 1 + q\right).$$

An induction argument and straightforward computations give

$$\begin{split} \bar{\zeta}_{k}\left(-r_{1},\ldots,-r_{k}\right) &= -\frac{1}{r_{k}+1}\sum_{q=0}^{r_{k}+1}\binom{r_{k}+1}{q}\left(-\mathcal{B}_{k}\right)^{q}\bar{\zeta}_{k-1}\left(-r_{1},\ldots,-r_{k-2},-r_{k-1}-r_{k}-1+q\right) \\ &= -\frac{1}{r_{k}+1}\sum_{q=0}^{r_{k}+1}\binom{r_{k}+1}{q}\left(-\mathcal{B}_{k}\right)^{q}\left(-1\right)^{r_{1}+\cdots+r_{k}+1-q}\mathcal{C}_{1}^{r_{1}+1}\cdots\mathcal{C}_{1,\ldots,k-1}^{r_{k-1}+r_{k}+2-q} \\ &= -\frac{(-1)^{r_{1}+\cdots+r_{k-1}}}{r_{k}+1}\mathcal{C}_{1}^{r_{1}+1}\cdots\mathcal{C}_{1,\ldots,k-1}^{r_{k-1}+1}\sum_{q=0}^{r_{k}+1}\binom{r_{k}+1}{q}\left(-\mathcal{B}_{k}\right)^{q}\left(-\mathcal{C}_{1,\ldots,k-1}\right)^{r_{k}+1-q} \\ &= -(-1)^{r_{1}+\cdots+r_{k}}\mathcal{C}_{1}^{r_{1}+1}\cdots\mathcal{C}_{1,\ldots,k-2}^{r_{k}-2}\mathcal{C}_{1,\ldots,k-1}^{r_{k}-1}\frac{\left(-\mathcal{C}_{1,\ldots,k-1}-\mathcal{B}_{k}\right)^{r_{k}+1}}{r_{k}+1} \\ &= (-1)^{r_{1}+\cdots+r_{k}}\mathcal{C}_{1}^{r_{1}+1}\cdots\mathcal{C}_{1,\ldots,k}^{r_{k}+1} \\ &= \prod_{i=1}^{k}\left(-1\right)^{r_{i}}\mathcal{C}_{1,\ldots,j}^{r_{j}+1}. \end{split}$$

The proof is complete.  $\Box$ 

It is surprising that both analytic continuations produce the same values. An explanation of this result is part of future work.

#### **Acknowledgements**

The authors would like to acknowledge referees for their valuable suggestions. The second author acknowledges the partial support of NSF-DMS 0713836. The work of the third author was partially funded by the iCODE Institute, a research project of the Idex Paris-Saclay.

#### References

Akiyama, S., Tanigawa, Y., 2001. Multiple zeta values at non-positive integers. Ramanujan J. 5, 327-351.

Akiyama, S., Egami, S., Tanigawa, Y., 2001. An analytic continuation of multiple zeta functions and their values at non-positive integers. Acta Arith. XCVIII, 107–116.

Broadhurst, D.J., 1986. Exploiting the 1,440-fold symmetry of the master two-loop diagram. Z. Phys. C 32, 249-253.

Ebrahimi-Fard, K., Manchon, D., Singer, J., 2002. Renormalization of *q*-regularized multiple zeta values. Lett. Math. Phys. 106, 365–380.

Fuks, B.A., 1963. Analytic Functions of Several Complex Variables. AMS.

Guo, L., Zhang, B., 2008. Renormalization of multiple zeta values. J. Algebra 319, 3770-3809.

Hoffman, M.E., 1992. Multiple harmonic series. Pac. J. Math. 152, 275-290.

Kytmanov, A.K., Myslivets, S.G., 2015. Multidimensional Integral Representations. Springer.

Manchon, D., Paycha, S., 2010. Nested sums of symbols and renormalized multiple zeta functions. Int. Math. Res. Not., 4628–4697.

Matsumoto, K., 2003. The analytic continuation and the asymptotic behavior of certain multiple zeta-functions I. J. Number Theory 101, 223–243.

Matsumoto, K., 2002. On the analytic continuation of various multiple zeta functions. In: Bennett, M.A., et al. (Eds.), Number Theory for the Millennium, vol. II. A.K. Peters, Natick, MA, pp. 417–440.

Sadaoui, B., 2014. Multiple zeta values at the non-positive integers. C. R. Acad. Sci. Paris, Ser. 1 352 (12), 12–352. pp. 977–984. Takamuki, T., 1999. The Kontsevich invariant and relations of multiple zeta values. Kobe J. Math. 16, 27–43.

Zagier, D., 1994. Values of zeta functions and their applications. Prog. Math. 120, 497-512.

Zhao, J., 2000. Analytic continuation of multiple zeta-functions. Proc. Am. Math. Soc. 128, 1275-1283.