

# Arborified Multiple Zeta Values



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**Abstract** We describe some particular finite sums of multiple zeta values which arise from J. Ecalle’s “arborification”, a process which can be described as a surjective Hopf algebra morphism from the Hopf algebra of decorated rooted forests onto a Hopf algebra of shuffles or quasi-shuffles. This formalism holds for both the iterated sum picture and the iterated integral picture. It involves a decoration of the forests by the positive integers in the first case, by only two colours in the second case.

**Keywords** Multiple zeta values · Rooted trees · Hopf algebras · Shuffle · Quasi-shuffle · Arborification

## 1 Introduction

Multiple zeta values are defined by the following nested sums:

$$\zeta(n_1, \dots, n_r) := \sum_{k_1 > k_2 > \dots > k_r \geq 1} \frac{1}{k_1^{n_1} \dots k_r^{n_r}}, \quad (1)$$

where the  $n_j$ ’s are positive integers. The nested sum (1) converges as long as  $n_1 \geq 2$ . The integer  $r$  is the *depth*, whereas the sum  $p := n_1 + \dots + n_r$  is the *weight*. Although the multiple zeta values of depth one and two were already known by L. Euler, the full set of multiple zeta values first appears in 1981 in a preprint of Jean Ecalle under the name “moule  $\zeta_{\leq}^{\bullet}$ ”, in the context of resurgence theory in complex analysis [9, Page 429], together with its companion  $\zeta_{\leq}^{\bullet}$  now known as the set of multiple star zeta values. The systematic study begins a decade later with the works of Hoffman [15] and Zagier [26]. It has been remarked by Kontsevich ([26], (see also the intriguing precursory Remark 4 on Page 431 in [9])) that multiple zeta values admit another representation by iterated integrals, namely:

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$$\zeta(n_1, \dots, n_r) = \int \cdots \int_{0 \leq u_p \leq \dots \leq u_1 \leq 1} \frac{du_1}{\varphi_1(u_1)} \cdots \frac{du_p}{\varphi_p(u_p)}, \tag{2}$$

with  $\varphi_j(u) = 1 - u$  if  $j \in \{n_1, n_1 + n_2, n_1 + n_2 + n_3, \dots, p\}$  and  $\varphi_j(u) = u$  otherwise. For later use we set:

$$f_0(u) := u, \quad f_1(u) := 1 - u.$$

Iterated integral representation (2) is the starting point to the modern approach in terms of mixed Tate motives over  $\mathbb{Z}$ , already outlined in [26] and widely developed in the literature since then [1–3, 7, 24]. Multiple zeta values verify a lot of polynomial relations with integer coefficients: the representation (1) by nested sums leads to *quasi-shuffle relations*, whereas representation (2) by iterated integrals leads to *shuffle relations*. A third family of relations, the *regularization relations*, comes from a subtle interplay between the first two families, involving divergent multiple zeta sums  $\zeta(1, n_2 \dots n_r)$ . A representative example of each family (in the order above) is given by:

$$\zeta(2, 3) + \zeta(3, 2) + \zeta(5) = \zeta(2)\zeta(3), \tag{3}$$

$$\zeta(2, 3) + 3\zeta(3, 2) + 6\zeta(4, 1) = \zeta(2)\zeta(3), \tag{4}$$

$$\zeta(2, 1) = \zeta(3). \tag{5}$$

It is conjectured that these three families include all possible polynomial relations between multiple zeta values. Note that the rationality of the quotient  $\frac{\zeta(2k)}{\pi^{2k}}$ , proved by L. Euler, does not yield supplementary polynomial identities. As an example,  $\zeta(2) = \frac{\pi^2}{6}$  and  $\zeta(4) = \frac{\pi^4}{90}$  yield  $2\zeta(2)^2 = 5\zeta(4)$ , a relation which can also be deduced from quasi-shuffle, shuffle and regularization relations.

It is convenient to write multiple zeta values in terms of words. In view of representations (1) and (2), this can be done in two different ways. We consider the two alphabets:

$$X := \{x_0, x_1\}, \quad Y := \{y_1, y_2, y_3, \dots\}, \tag{6}$$

and we denote by  $X^*$  (resp.  $Y^*$ ) the set of words with letters in  $X$  (resp.  $Y$ ). The vector space  $\mathbb{Q}\langle X \rangle$  freely generated by  $X^*$  is a commutative algebra for the *shuffle product*, which is defined by:

$$(v_1 \cdots v_p) \sqcup (v_{p+1} \cdots v_{p+q}) := \sum_{\sigma \in \text{Sh}(p,q)} v_{\sigma_1}^{-1} \cdots v_{\sigma_{p+q}}^{-1} \tag{7}$$

with  $v_j \in X$ ,  $j \in \{1, \dots, p + q\}$ . Here,  $\text{Sh}(p, q)$  is the set of  $(p, q)$ -*shuffles*, i.e. permutations  $\sigma$  of  $\{1, \dots, p + q\}$  such that  $\sigma_1 < \dots < \sigma_p$  and  $\sigma_{p+1} < \dots < \sigma_{p+q}$ . The vector space  $\mathbb{Q}\langle Y \rangle$  freely generated by  $Y^*$  is a commutative algebra for the *quasi-shuffle product*, which is defined as follows: a  $(p, q)$ -*quasi-shuffle of type  $r$*

is a surjection  $\sigma : \{1, \dots, p + q\} \twoheadrightarrow \{1, \dots, p + q - r\}$  such that  $\sigma_1 < \dots < \sigma_p$  and  $\sigma_{p+1} < \dots < \sigma_{p+q}$ . Denoting by  $\text{Qsh}(p, q; r)$  the set of  $(p, q)$ -quasi-shuffles of type  $r$ , the formula for the quasi-shuffle product  $\mathfrak{H}$  is:

$$(w_1 \cdots w_p) \mathfrak{H} (w_{p+1} \cdots w_{p+q}) := \sum_{r \geq 0} \sum_{\sigma \in \text{Qsh}(p, q; r)} w_1^\sigma \cdots w_{p+q-r}^\sigma \tag{8}$$

with  $w_j \in Y, j \in \{1, \dots, p + q\}$ , and where  $w_j^\sigma$  is the *internal product* of the letters in the set  $\sigma^{-1}(\{j\})$ , which contains one or two elements. The internal product is defined by  $[y_k y_l] := y_{k+l}$ .

We denote by  $Y_{\text{conv}}^*$  the submonoid of words  $w = w_1 \cdots w_r$  with  $w_1 \neq y_1$ , and we set  $X_{\text{conv}}^* = x_0 X^* x_1$ . An injective monoid morphism is given by changing letter  $y_n$  into the word  $x_0^{n-1} x_1$ , namely:

$$\begin{aligned} \mathfrak{s} : Y^* &\longrightarrow X^* \\ y_{n_1} \cdots y_{n_r} &\longmapsto x_0^{n_1-1} x_1 \cdots x_0^{n_r-1} x_1, \end{aligned}$$

and restricts to a monoid isomorphism from  $Y_{\text{conv}}^*$  onto  $X_{\text{conv}}^*$ . As notation suggests,  $Y_{\text{conv}}^*$  and  $X_{\text{conv}}^*$  are two convenient ways to symbolize convergent multiple zeta values through representations (1) and (2) respectively. The following notations are commonly adopted:

$$\zeta_{\mathfrak{H}}(y_{n_1} \cdots y_{n_r}) := \zeta(n_1, \dots, n_r), \tag{9}$$

$$\zeta_{\mathfrak{H}}(x_{e_1} \cdots x_{e_p}) := \int \cdots \int_{0 \leq u_p \leq \dots \leq u_1 \leq 1} \frac{du_1}{f_{e_1}(u_1)} \cdots \frac{du_p}{f_{e_p}(u_p)}, \tag{10}$$

and extended to finite linear combinations of convergent words by linearity. In particular we have:

$$\zeta(n_1, \dots, n_r) = \zeta_{\mathfrak{H}}(x_0 x_1^{n_1} \cdots x_0 x_1^{n_r}), \tag{11}$$

hence the relation:

$$\zeta_{\mathfrak{H}} = \zeta_{\mathfrak{H}} \circ \mathfrak{s}$$

is obviously verified. The quasi-shuffle relations then write:

$$\zeta_{\mathfrak{H}}(w \mathfrak{H} w') = \zeta_{\mathfrak{H}}(w) \zeta_{\mathfrak{H}}(w') \tag{12}$$

for any  $w, w' \in Y_{\text{conv}}^*$ , whereas the shuffle relations write:

$$\zeta_{\mathfrak{H}}(v \mathfrak{H} v') = \zeta_{\mathfrak{H}}(v) \zeta_{\mathfrak{H}}(v') \tag{13}$$

for any  $v, v' \in X_{\text{conv}}^*$ . By assigning an indeterminate value  $\theta$  to  $\zeta(1)$  and setting  $\zeta_{\mathfrak{H}}(y_1) = \zeta_{\mathfrak{H}}(x_1) = \theta$ , it is possible to extend  $\zeta_{\mathfrak{H}}$ , resp.  $\zeta_{\mathfrak{H}}$ , to all words in  $Y^*$ , resp. to  $X^* x_1$ , such that (12), resp. (13), still holds. It is also possible to extend  $\zeta_{\mathfrak{H}}$  to a

map defined on  $X^*$  by assigning an indeterminate value  $\theta'$  to  $\zeta_{\mathbb{H}}(x_0)$ , such that (13) is still valid. We will stick to  $\theta' = \theta$  for symmetry reasons, reflecting the following formal equality between two infinite quantities:

$$\int_0^1 \frac{dt}{t} = \int_0^1 \frac{dt}{1-t}.$$

It is easy to show that for any word  $v \in X^*$  or  $w \in Y^*$ , the expressions  $\zeta_{\mathbb{H}}(v)$  and  $\zeta_{\mathbb{H}}(w)$  are polynomial with respect to  $\theta$ . It is no longer true that extended  $\zeta_{\mathbb{H}}$  coincides with extended  $\zeta_{\mathbb{H}} \circ \mathfrak{s}$ , but the defect can be explicitly written:

**Theorem 1** (Boutet de Monvel and Zagier [26]) *There exists an infinite-order invertible differential operator  $\rho : \mathbb{R}[\theta] \rightarrow \mathbb{R}[\theta]$  such that*

$$\zeta_{\mathbb{H}} \circ \mathfrak{s} = \rho \circ \zeta_{\mathbb{H}}. \tag{14}$$

The operator  $\rho$  is explicitly given by the series:

$$\rho = \exp \left( \sum_{n \geq 2} \frac{(-1)^n \zeta(n)}{n} \left( \frac{d}{d\theta} \right)^n \right). \tag{15}$$

In particular,  $\rho(1) = 1$ ,  $\rho(\theta) = \theta$ , and more generally  $\rho(P) - P$  is a polynomial of degree  $\leq d - 2$  if  $P$  is of degree  $d$ , hence  $\rho$  is invertible. A proof of Theorem 1 can be read in numerous references, e.g. [5, 17, 21]. Any word  $w \in Y_{\text{conv}}^*$  gives rise to Hoffman’s regularization relation:

$$\zeta_{\mathbb{H}}(x_1 \mathbb{H} \mathfrak{s}(w) - \mathfrak{s}(y_1 \mathbb{H} w)) = 0, \tag{16}$$

which is a direct consequence of Theorem 1. The linear combination of words involved above is convergent, hence (16) is a relation between convergent multiple zeta values, although divergent ones have been used to establish it. The simplest regularization relation (5) is nothing but (16) applied to the word  $w = y_2$ .

Rooted trees can enrich the picture in two ways: first of all, considering a rooted tree  $t$  with set of vertices  $\mathcal{V}(t)$  and decoration  $n_v \in \mathbb{Z}_{>0}$ ,  $v \in \mathcal{V}(t)$ , we define the associated *contracted arborified multiple zeta value* by:

$$\zeta^{\mathcal{T}}(t) := \sum_{k \in D_t} \prod_{v \in \mathcal{V}(t)} \frac{1}{k_v^{n_v}}, \tag{17}$$

where  $D_t$  is made of those maps  $v \mapsto k_v \in \mathbb{Z}_{>0}$  such that  $k_v < k_w$  if and only if there is a path from the root to  $w$  through  $v$ . The sum (17) is convergent as long as  $n_v \geq 2$  if  $v$  is a leaf of  $t$ . The definition is multiplicatively extended to rooted forests. A similar definition can be introduced starting from the integral representation (2): considering

a rooted tree  $\tau$  with set of vertices  $\mathcal{V}(\tau)$  and decoration  $e_v \in \{0, 1\}$ ,  $v \in \mathcal{V}(\tau)$ , we define the associated *arborified multiple zeta value* by:

$$\zeta^T(\tau) := \int_{u \in \Delta_\tau} \prod_{v \in \mathcal{V}(\tau)} \frac{du_v}{f_{e_v}(u_v)}, \tag{18}$$

where  $\Delta_\tau \subset [0, 1]^{|\mathcal{V}(\tau)|}$  is made of those maps  $v \mapsto u_v \in [0, 1]$  such that  $u_v \leq u_w$  if and only if there is a path from the root to  $w$  through  $v$ . The integral (18) is convergent as long as  $e_v = 1$  if  $v$  is the root of  $\tau$  and  $e_v = 0$  if  $v$  is a leaf of  $\tau$ . A multiplicative extension to two-coloured rooted forests will also be considered. A further extension of multiple zeta values to more general finite posets than rooted forests, in this non-contracted form, recently appeared in a paper by Yamamoto [25], see also [18]. We give a brief account of these ‘‘posetified’’ multiple zeta values in Sect. 6.

Arborified and contracted arborified multiple zeta values are finite linear combinations of ordinary ones. For example we have :

$$\zeta^{\mathcal{F}} \left( \begin{array}{c} \circlearrowleft n_1 \quad \circlearrowleft n_2 \\ \diagdown \quad \diagup \\ \circlearrowleft n_3 \end{array} \right) = \zeta(n_1, n_2, n_3) + \zeta(n_2, n_1, n_3) + \zeta(n_1 + n_2, n_3)$$

and, choosing white for colour 0 and black for colour 1:

$$\begin{aligned} \zeta^T \left( \begin{array}{c} \circ \\ \circ \\ \bullet \end{array} \right) &= 2\zeta(3, 1) + \zeta(2, 2), \\ \zeta^T \left( \begin{array}{c} \circ \\ \circ \\ \bullet \end{array} \right) &= 3\zeta(4). \end{aligned}$$

The terminology comes from J. Ecalle’s *arborification*, a transformation which admits a ‘‘simple’’ and a ‘‘contracting’’ version [10, 11]. This transformation is best understood in terms of a canonical surjective morphism from Butcher-Connes-Kreimer Hopf algebra of rooted forests onto a corresponding shuffle Hopf algebra (quasi-shuffle Hopf algebra for the contracting arborification) [13].

The paper is organized as follows: after a reminder on shuffle and quasi-shuffle Hopf algebras, we describe the two versions of arborification in some detail, and we describe a possible transformation from contracted arborified to arborified multiple zeta values, which can be seen as an arborified version of the map  $\mathfrak{s}$  from words in  $Y^*$  into words in  $X^*$ . A more natural version of this arborified  $\mathfrak{s}$  with respect to the tree structures is still to be found. We finally give in Sect. 6 an account of the more general poset multiple zeta values in both simple and contracting versions, and we interpret the restricted sum formula of [12, 23] in terms of simple poset multiple zeta values.

## 2 Shuffle and Quasi-Shuffle Hopf Algebras

Let  $V$  be any commutative algebra on a base field  $k$  of characteristic zero. The product on  $V$  will be denoted by  $(a, b) \mapsto [ab]$ . This algebra is not supposed to be unital: in particular any vector space can be considered as a commutative algebra with trivial product  $(a, b) \mapsto [ab] = 0$ . The associated *quasi-shuffle Hopf algebra* is  $(T(V), \mathfrak{H}, \Delta)$ , where  $(T(V), \Delta)$  is the tensor coalgebra:

$$T(V) = \bigoplus_{k \geq 0} V^{\otimes k}.$$

The decomposable elements of  $V^{\otimes k}$  will be denoted by  $v_1 \cdots v_k$  with  $v_j \in V$ . The coproduct  $\Delta$  is the deconcatenation coproduct:

$$\Delta(v_1 \cdots v_k) := \sum_{r=0}^k v_1 \cdots v_r \otimes v_{r+1} \cdots v_k. \tag{19}$$

The quasi-shuffle product  $\mathfrak{H}$  is given for any  $v_1, \dots, v_{p+q}$  by:

$$(v_1 \cdots v_p) \mathfrak{H} (v_{p+1} \cdots v_{p+q}) := \sum_{r \geq 0} \sum_{\sigma \in \text{Qsh}(p, q; r)} v_1^\sigma \cdots v_{p+q-r}^\sigma \tag{20}$$

with  $v_j \in Y, j \in \{1, \dots, p + q\}$ , and where  $v_j^\sigma$  is the internal product of the letters in the set  $\sigma^{-1}(\{j\})$ , which contains one or two elements. Note that if the internal product vanishes, only ordinary shuffles (i.e. quasi-shuffles of type  $r = 0$ ) do contribute to the quasi-shuffle product, which specializes to the shuffle product  $\mathfrak{H}$  in this case. The tensor coalgebra endowed with the quasi-shuffle product  $\mathfrak{H}$  is a Hopf algebra which, remarkably enough, does not depend on the particular choice of the internal product [16]. An explicit Hopf algebra isomorphism  $\exp$  from  $(T(V), \mathfrak{H}, \Delta)$  onto  $(T(V), \mathfrak{H}, \Delta)$  is given in [16]. Although we won't use it, let us recall its expression: let  $\mathcal{P}(k)$  be the set of compositions of the integer  $k$ , i.e. the set of sequences  $I = (i_1, \dots, i_r)$  of positive integers such that  $i_1 + \dots + i_r = k$ . For any  $u = v_1 \dots v_k \in T(V)$  and any composition  $I = (i_1, \dots, i_r)$  of  $k$  we set:

$$I[u] := [v_1 \dots v_{i_1}].[v_{i_1+1} \dots v_{i_1+i_2}] \dots [v_{i_1+\dots+i_{r-1}+1} \dots v_k].$$

Then:

$$\exp u = \sum_{I=(i_1, \dots, i_r) \in \mathcal{P}(k)} \frac{1}{i_1! \dots i_r!} I[u].$$

Moreover ([16], lemma 2.4), the inverse log of exp is given by :

$$\log u = \sum_{I=(i_1, \dots, i_r) \in \mathcal{P}(k)} \frac{(-1)^{k-r}}{i_1 \dots i_r} I[u].$$

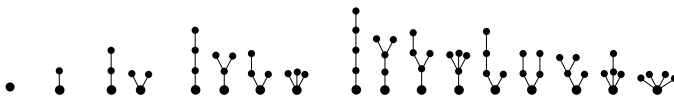
For example for  $v_1, v_2, v_3 \in V$  we have:

$$\begin{aligned} \exp v_1 &= v_1, \quad \log v_1 = v_1, \\ \exp(v_1 v_2) &= v_1 v_2 + \frac{1}{2}[v_1 v_2], \quad \log(v_1 v_2) = v_1 v_2 - \frac{1}{2}[v_1 v_2], \\ \exp(v_1 v_2 v_3) &= v_1 v_2 v_3 + \frac{1}{2}([v_1 v_2]v_3 + v_1[v_2 v_3]) + \frac{1}{6}[v_1 v_2 v_3], \\ \log(v_1 v_2 v_3) &= v_1 v_2 v_3 - \frac{1}{2}([v_1 v_2]v_3 + v_1[v_2 v_3]) + \frac{1}{3}[v_1 v_2 v_3]. \end{aligned}$$

Going back to the notations of the introduction,  $\mathbb{Q}\langle Y \rangle$  is the quasi-shuffle Hopf algebra associated to the algebra  $tk[t]$  of polynomials without constant terms, whereas  $\mathbb{Q}\langle X \rangle$  is the shuffle Hopf algebra associated with the two-dimensional vector space spanned by  $X$ .

### 3 The Butcher-Connes-Kreimer Hopf Algebra of Decorated Rooted Trees

Let  $\mathcal{D}$  be a set. A *rooted tree* is an oriented (non planar) graph with a finite number of vertices, among which one is distinguished and called the *root*, such that any vertex admits exactly one incoming edge, except the root which has no incoming edges. A  *$\mathcal{D}$ -decorated rooted tree* is a rooted tree  $t$  together with a map from its set of vertices  $\mathcal{V}(t)$  into  $\mathcal{D}$ . Here is the list of (non-decorated) rooted trees up to five vertices:



A  *$\mathcal{D}$ -decorated rooted forest* is a finite collection of  $\mathcal{D}$ -decorated rooted trees, with possible repetitions. The empty set is the forest containing no trees, and is denoted by  $\mathbf{1}$ . For any  $d \in \mathcal{D}$ , the *grafting operator*  $B_+^d$  takes any forest and changes it into a tree by grafting all components onto a common root decorated by  $d$ , with the convention  $B_+^d(\mathbf{1}) = \bullet_d$ .

Let  $\mathcal{T}^{\mathcal{D}}$  denote the set of nonempty rooted trees and let  $\mathcal{H}_{\text{BCK}}^{\mathcal{D}} = k[\mathcal{T}^{\mathcal{D}}]$  be the free commutative unital algebra generated by elements of  $\mathcal{T}^{\mathcal{D}}$ . We identify a product of trees with the forest containing these trees. Therefore the vector space underlying

$\mathcal{H}_{\text{BCK}}^{\mathcal{D}}$  is the linear span of rooted forests. This algebra is a graded and connected Hopf algebra, called the *Hopf algebra of  $\mathcal{D}$ -decorated rooted trees*, with the following structure: the grading is given by the number of vertices, and the coproduct on a rooted forest  $u$  is described as follows [14, 20]: the set  $\mathcal{V}(u)$  of vertices of a forest  $u$  is endowed with a partial order defined by  $x \leq y$  if and only if there is a path from a root to  $y$  passing through  $x$ . Any subset  $W$  of  $\mathcal{V}(u)$  defines a *subforest*  $u|_W$  of  $u$  in an obvious manner, i.e. by keeping the edges of  $u$  which link two elements of  $W$ . The coproduct is then defined by:

$$\Delta(u) = \sum_{\substack{V \sqcup W = \mathcal{V}(u) \\ W < V}} u|_V \otimes u|_W. \tag{21}$$

Here the notation  $W < V$  means that  $y < x$  for any vertex  $x$  in  $V$  and any vertex  $y$  in  $W$  such that  $x$  and  $y$  are comparable. Such a couple  $(V, W)$  is also called an *admissible cut*, with *crown* (or *pruning*)  $u|_V$  and *trunk*  $u|_W$ . We have for example:

$$\begin{aligned} \Delta(\bullet) &= \bullet \otimes \mathbf{1} + \mathbf{1} \otimes \bullet + \bullet \otimes \bullet \\ \Delta(\curvearrowright) &= \curvearrowright \otimes \mathbf{1} + \mathbf{1} \otimes \curvearrowright + 2 \bullet \otimes \bullet + \bullet \otimes \bullet \end{aligned}$$

The counit is  $\varepsilon(\mathbf{1}) = 1$  and  $\varepsilon(u) = 0$  for any non-empty forest  $u$ . The coassociativity of the coproduct is easily checked using the following formula for the iterated coproduct:

$$\tilde{\Delta}^{n-1}(u) = \sum_{\substack{V_1 \sqcup \dots \sqcup V_n = \mathcal{V}(u) \\ V_n < \dots < V_1}} u|_{V_1} \otimes \dots \otimes u|_{V_n}.$$

The notation  $V_n < \dots < V_1$  is to be understood as  $V_i < V_j$  for any  $i > j$ , with  $i, j \in \{1, \dots, n\}$ .

This Hopf algebra first appeared in the work of Dür in 1986 [8]. Its dual algebra appears in [10] (Page 81 therein). It has been rediscovered and intensively studied by Kreimer in 1998 [19], as the Hopf algebra describing the combinatorial part of the BPHZ renormalization procedure of Feynman graphs in a scalar  $\varphi^3$  quantum field theory. Its group of characters:

$$G_{\text{BCK}}^{\mathcal{D}} = \text{Hom}_{\text{alg}}(\mathcal{H}_{\text{BCK}}^{\mathcal{D}}, k) \tag{22}$$

is known as the *Butcher group* and plays a key role in approximation methods in numerical analysis [4]. Connes and Kreimer also proved in [6] that the operators  $B_+^d$  satisfy the property

$$\Delta(B_+^d(t_1 \dots t_n)) = B_+^d(t_1 \dots t_n) \otimes \mathbf{1} + (\text{Id} \otimes B_+^d) \circ \Delta(t_1 \dots t_n), \tag{23}$$

for any  $t_1, \dots, t_n \in \mathcal{T}$ . This means that  $B_+^d$  is a 1-cocycle in the Hochschild cohomology of  $\mathcal{H}_{\text{BCK}}^{\mathcal{D}}$  with values in  $\mathcal{H}_{\text{BCK}}^{\mathcal{D}}$ .



### 4 Simple and Contracting Arborification

The Hopf algebra of decorated rooted forests enjoys the following universal property (see e.g. [14]): let  $\mathcal{D}$  be a set, let  $\mathcal{H}$  be a graded Hopf algebra, and, for any  $d \in \mathcal{D}$ , let  $L^d : \mathcal{H} \rightarrow \mathcal{H}$  be a Hochschild one-cocycle, i.e. a linear map such that:

$$\Delta(L^d(x)) = L^d(x) \otimes \mathbf{1}_{\mathcal{H}} + (\text{Id} \otimes L^d) \circ \Delta(x). \tag{24}$$

Then there exists a unique Hopf algebra morphism  $\Phi : \mathcal{H}_{\text{BCK}}^{\mathcal{D}} \rightarrow \mathcal{H}$  such that:

$$\Phi \circ B_+^d = L^d \circ \Phi \tag{25}$$

for any  $d \in \mathcal{D}$ . Now let  $V$  be a commutative algebra, let  $(T(V), \mathfrak{H}, \Delta)$  be the corresponding quasi-shuffle Hopf algebra, let  $(e_d)_{d \in \mathcal{D}}$  be a linear basis of  $V$ , and let  $L^d : T(V) \rightarrow T(V)$  the right concatenation by  $e_d$ , defined by:

$$L^d(v_1 \dots v_k) := v_1 \dots v_k e_d. \tag{26}$$

One can easily check, due to the particular form of the deconcatenation coproduct, that  $L^d$  verifies the one-cocycle condition (24). The *contracting arborification* of the quasi-shuffle Hopf algebra above is the unique Hopf algebra morphism

$$\alpha_V : \mathcal{H}_{\text{BCK}}^{\mathcal{D}} \twoheadrightarrow (T(V), \mathfrak{H}, \Delta) \tag{27}$$

such that  $\alpha_V \circ B_+^d = L^d \circ \alpha_V$  for any  $d \in \mathcal{D}$ . The map  $\alpha_V$  sends any decorated forest to the sum of all its linear extensions, taking contractions into account (see Example (30) below). It is obviously surjective, since the word  $w = e_{d_1} \dots e_{d_r}$  can be obtained as the image of the ladder  $\ell_Y(w)$  with  $r$  vertices decorated by  $d_1, \dots, d_r$  from top to bottom. This map is invariant under linear base changes. For the shuffle algebra (i.e. when the internal product on  $V$  is set to zero), the corresponding Hopf algebra morphism  $\alpha_V$  is called *simple arborification*, and the corresponding section will be denoted by  $\ell_X$  (see Examples (31) and (32) below).

Let us apply this construction to multiple zeta values (the base field  $k$  being the field  $\mathbb{Q}$  of rational numbers): we denote by  $\alpha_X$  (resp.  $\alpha_Y$ ) the simple (resp. contracting) arborification from  $\mathcal{H}_{\text{BCK}}^X$  onto  $\mathbb{Q}\langle X \rangle$  (resp. from  $\mathcal{H}_{\text{BCK}}^Y$  onto  $\mathbb{Q}\langle Y \rangle$ ). The maps  $\zeta_{\mathfrak{H}}$  and  $\zeta_{\mathfrak{H}}$  defined in the introduction are characters of the (Hopf) algebras  $\mathbb{Q}\langle X \rangle$  and  $\mathbb{Q}\langle Y \rangle$  respectively, with values in the algebra  $\mathbb{R}[\theta]$ . The simple and contracted arborified multiple zeta values are then respectively given by:

$$\begin{aligned} \zeta_{\mathfrak{H}}^T : \mathcal{H}_{\text{BCK}}^X &\longrightarrow \mathbb{R}[\theta] \\ \tau &\longmapsto \zeta_{\mathfrak{H}}^T(\tau) = \zeta_{\mathfrak{H}} \circ \alpha_X(\tau). \end{aligned} \tag{28}$$

and:

$$\begin{aligned} \zeta_{\mathfrak{m}}^{\mathcal{F}} : \mathcal{H}_{\text{BCK}}^Y &\longrightarrow \mathbb{R}[\theta] \\ t &\longmapsto \zeta_{\mathfrak{m}}^{\mathcal{F}}(t) = \zeta_{\mathfrak{m}} \circ \mathfrak{a}_Y(t). \end{aligned} \tag{29}$$

They are obviously characters of  $\mathcal{H}_{\text{BCK}}^X$  and  $\mathcal{H}_{\text{BCK}}^Y$  respectively, and respectively coincide with the maps  $\zeta^T$  and  $\zeta^{\mathcal{F}}$  defined in the introduction. This last statement comes from the fact that, for any  $X$ -decorated forest  $\tau$ , the domain  $\Delta_\tau$  can be decomposed in a union of simplices the same way  $\mathfrak{a}_X(\tau)$  is decomposed as the sum of its linear extensions, and similarly with contracting arborification  $\mathfrak{a}_Y$  for any  $Y$ -decorated forest  $t$ , taking diagonals in  $D_t$  into account. Looking back at the examples given there we have:

$$\mathfrak{a}_Y \left( \begin{array}{c} \textcircled{n_1} \quad \textcircled{n_2} \\ \diagdown \quad \diagup \\ \textcircled{n_3} \end{array} \right) = y_{n_1}y_{n_2}y_{n_3} + y_{n_2}y_{n_1}y_{n_3} + y_{n_1+n_2}y_{n_3} \tag{30}$$

and

$$\mathfrak{a}_X \left( \begin{array}{c} \circ \\ | \\ \bullet \\ | \\ \bullet \end{array} \right) = 2x_0x_0x_1x_1 + x_0x_1x_0x_1, \tag{31}$$

$$\mathfrak{a}_X \left( \begin{array}{c} \circ \\ | \\ \bullet \\ | \\ \bullet \\ | \\ \bullet \end{array} \right) = 3x_0x_0x_0x_1. \tag{32}$$

### 5 Arborification of the Map $\mathfrak{s}$

We are looking for a map  $\mathfrak{s}^T$  which makes the following diagram commutative:

$$\begin{array}{ccc} \mathcal{H}_{\text{BCK}}^Y & \xrightarrow{\mathfrak{s}^T} & \mathcal{H}_{\text{BCK}}^X \\ \downarrow \mathfrak{a}_Y & & \downarrow \mathfrak{a}_X \\ \mathbb{Q}\langle Y \rangle & \xrightarrow{\mathfrak{s}} & \mathbb{Q}\langle X \rangle \end{array}$$

An obvious answer to this problem is given by:

$$\mathfrak{s}^T = \ell_X \circ \mathfrak{s} \circ \mathfrak{a}_Y,$$

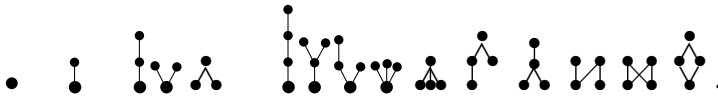
where  $\ell_X$  is the section of  $\mathfrak{a}_X$  described in the previous section. It has the drawback of completely destroying the geometry of trees: indeed, any  $Y$ -decorated forest is mapped on a linear combination of  $X$ -decorated ladders. We are then looking for a more natural map with respect to the tree structures, which makes the diagram above commute, or at least the outer square of the diagram below:

$$\begin{array}{ccc}
 \mathcal{H}_{\text{BCK}}^Y & \xrightarrow{s^T} & \mathcal{H}_{\text{BCK}}^X \\
 \downarrow \alpha_Y & & \downarrow \alpha_X \\
 \mathbb{Q}\langle Y \rangle & \xrightarrow{s} & \mathbb{Q}\langle X \rangle \\
 \downarrow \zeta_{\text{III}} & & \downarrow \zeta_{\text{III}} \\
 \mathbb{R}[\theta] & \xrightarrow{\rho} & \mathbb{R}[\theta]
 \end{array}
 \begin{array}{l}
 \zeta_{\text{III}}^T \curvearrowright \\
 \zeta_{\text{III}}^T \curvearrowleft
 \end{array}$$

This interesting problem remains open.

### 6 Poset Multiple Zeta Values

A rooted forest is nothing but a particular finite poset in which each non-minimal element (i.e. each vertex different from a root)  $x$  has a unique predecessor, i.e. there exists a unique  $y < x$  such that for any  $z$  with  $y \leq z \leq x$ , one has  $z = x$  or  $z = y$ . It turns out that most of the concepts previously defined still make sense without this last condition. First of all, identities (17) and (18) define real numbers for any finite poset  $t$  (resp.  $\tau$ ) respectively decorated by  $Y$  and  $X$ , respectively named *contracted poset multiple zeta values* and *simple poset multiple zeta value*. Connected (non-decorated) posets up to four vertices are given by:



We have for example:

$$\zeta^T \left( \begin{array}{c} \circ_{n_1} \\ / \quad \backslash \\ \circ_{n_2} \quad \circ_{n_3} \\ \backslash \quad / \\ \circ_{n_4} \end{array} \right) = \zeta(n_1, n_2, n_3, n_4) + \zeta(n_1, n_3, n_2, n_4) + \zeta(n_1, n_2 + n_3, n_4)$$

and

$$\zeta^T \left( \begin{array}{c} \circ \\ / \quad \backslash \\ \circ \quad \circ \\ \backslash \quad / \\ \circ \end{array} \right) = \zeta(3, 1) + \zeta(2, 2).$$

Next, for any set  $D$ , the linear span of isomorphism classes of  $D$ -decorated posets is a graded connected commutative Hopf algebra  $\mathcal{H}_P^D$ . The product is given by disjoint union, and the coproduct is still given by Formula (21). It is well-known that  $\mathcal{H}_P^D$  is a commutative incidence Hopf algebra: see [22, Paragraph 16], taking for  $\mathcal{F}$  the family of all finite posets with the notations therein. The forest Hopf algebra  $\mathcal{H}_{\text{BCK}}^D$  is a Hopf

subalgebra of  $\mathcal{H}_p^D$ . The simple arborification  $\mathfrak{a}_X : \mathcal{H}_{BCK}^X \rightarrow (T(X), \mathfrak{M}, \Delta)$  extends to a surjective Hopf algebra morphism  $\mathfrak{p}_X : \mathcal{H}_p^X \rightarrow (T(X), \mathfrak{M}, \Delta)$  and, similarly, the contracting arborification  $\mathfrak{a}_Y : \mathcal{H}_{BCK}^Y \rightarrow (T(Y), \mathfrak{M}, \Delta)$  extends to a surjective Hopf algebra morphism  $\mathfrak{p}_Y : \mathcal{H}_p^Y \rightarrow (T(Y), \mathfrak{M}, \Delta)$ .

The “posetization” map  $\mathfrak{p}_X$  and its contracting version  $\mathfrak{p}_Y$  still map a poset on the sum of all its linear extensions, moreover taking contraction terms into account in the case of  $\mathfrak{p}_Y$ . The fact that both are Hopf algebra morphisms can be checked by a routine computation.

The canonical involution  $\iota$  on the set of finite posets is given by reversing the order: for example,

$$\iota(\text{poset}) = \text{poset}.$$

The duality involution  $\sigma$  on the set of  $X$ -decorated posets is given by both applying  $\iota$  and switching the two colours, i.e. exchanging 0 and 1. The duality relations for multiple zeta values extends to poset multiple zeta values as follows:

$$\zeta^T(\tau) = \zeta^T \circ \sigma(\tau). \tag{33}$$

Poset multiple zeta values recently appeared (in the simple form only) in a paper by Yamamoto [25], as well as in another paper of the same author together with Kaneko [18]. Let us mention that the restricted sum formula of [12], (see [23], formula (2) therein) can be understood as an equality between two poset multiple zeta values (in the simple version) involving “kite-shaped” posets, namely:

$$\zeta^T(A_{a,b,c}) = \zeta^T(B_{a,b,c}), \tag{34}$$

where  $a, b, c$  are three non-negative integers, and where  $A_{a,b,c}$  and  $B_{a,b,c}$  are defined as follows:

- $A_{a,b,c}$  has a unique white maximum linked to two ladders, the first made of  $c$  white vertices, the second made of  $b$  black vertices. Both join to a black ladder (the tail, pointing downwards) of length  $a + 1$ .
- $B_{a,b,c}$  has a unique black minimum linked to two ladders, the first made of  $b$  white vertices, the second made of  $a$  black vertices. Both join to a white ladder (the tail, pointing upwards) of length  $c + 1$ .

Both posets defined above have total number of vertices equal to  $a + b + c + 2$ . From (33) and (34), we immediately get:

$$\zeta^T(A_{a,b,c}) = \zeta^T(A_{c,b,a}). \tag{35}$$

Finally, the question asked in Sect. 5 makes also sense in the poset context, replacing the two Hopf algebras  $\mathcal{H}_{BCK}^X$  and  $\mathcal{H}_{BCK}^Y$  respectively by  $\mathcal{H}_p^X$  and  $\mathcal{H}_p^Y$ .

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