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# Algorithmic and combinatoric aspects of multiple harmonic sums

## Christian Costermans and Jean-Yves Enjalbert and Hoang Ngoc Minh

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Ordinary generating series of *multiple* harmonic sums admit a *full* singular expansion in the basis of functions  $\{(1-z)^{\alpha}\log^{\beta}(1-z)\}_{\alpha\in\mathbb{Z},\beta\in\mathbb{N}}$ , near the singularity z=1. A *constructive* proof of this result is given, and, by *combinatoric* aspects, an explicit evaluation of Taylor coefficients of functions in some *polylogarithmic* algebra is obtained. In particular, the *asymptotic expansion* of multiple harmonic sums is easily deduced.

Keywords: polylogarithms, polyzêtas, multiple harmonic sums, singular expansion, shuffle algebra, Lyndon words

#### 1 Introduction

Hierarchical data structure occur in numerous domains, like computer graphics, image processing or biology (pattern matching). Among them, quadtrees, whose construction is based on a recursive definition of space, constitute a classical data structure for storing and accessing collection of points in multidimensional space. Their characteristics (depth of a node, number of nodes in a given subtree, number of leaves) are studied by Laforest [12], with probabilistic tools. In particular, she shows, for a quadtree of size N in a d-dimension space, that the probability  $\pi_{N,k}$  for the first subtree to have size k can be expressed as an algebraic combination of j-th order harmonic numbers  $H_j(N)$  and  $H_j(k)$ ,  $j \geq 1$ , defined by

$$H_j(n) = \sum_{m=1}^n \frac{1}{m^j}.$$
 (1)

For instance, for d = 3, one has

$$\pi_{N,k} = \frac{[H_1(N) - H_1(k)]^2 + H_2(N) - H_2(k)}{2N}.$$
 (2)

Flajolet et al. [2] give this general expression for the splitting probability

$$\pi_{N,k} = \sum_{N > i_1 \dots > i_{d-1} > k} \frac{1}{i_1 \dots i_{d-1}}.$$
(3)

The probability  $\pi_{N,k}$  appears as a particular case of the following sum  $A_s(N)$  associated to the *multi-index*  $s = (s_1, \ldots, s_r)$ , which is strongly related to multiple harmonic sums  $H_s(N)$ :

$$A_{\mathbf{s}}(N) = \sum_{N \ge n_1 \ge \dots \ge n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}} \quad \text{and} \quad H_{\mathbf{s}}(N) = \sum_{N \ge n_1 > \dots > n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}}. \tag{4}$$

Let us note that there exist explicit relations, given by Hoffman [10] between the  $A_s(N)$  and  $H_s(N)$ . Indeed, let  $\mathrm{Comp}(n)$  be the *set of compositions* of n, i.e. sequences  $(i_1,\ldots,i_r)$  of positive integers summing to n. If  $I=(i_1,\ldots,i_r)$  (resp.  $J=(j_1,\ldots,j_p)$ ) is a composition of n (resp. of r) then  $J\circ I=(i_1+\ldots+i_{j_1},i_{j_1+1}+\ldots+i_{j_1+j_2},\ldots,i_{k-j_p+1}+\ldots+i_k)$  is a composition of n. By Möbius inversion, one has

$$A_{\mathbf{s}}(N) = \sum_{J \in Comp(r)} H_{J \circ \mathbf{s}}(N) \quad \text{and} \quad H_{\mathbf{s}}(N) = \sum_{J \in Comp(r)} (-1)^{l(J)-r} A_{J \circ \mathbf{s}}(N), \tag{5}$$

where l(J) is the number of parts of J.

**Example 1.** For s = (1, 1, 1), since the set of compositions of 3 is  $\{(1, 1, 1), (1, 2), (2, 1), (3)\}$ , we get

$$\mathbf{A}_{1,1,1}(N) \ = \ \mathbf{H}_{1,1,1}(N) + \mathbf{H}_{1,2}(N) + \mathbf{H}_{2,1}(N) + \mathbf{H}_{3}(N),$$

$$H_{1,1,1}(N) = A_{1,1,1}(N) - A_{1,2}(N) - A_{2,1}(N) + A_{3}(N).$$

Therefore, the  $A_s(N)$  are  $\mathbb{Z}$ -linear combinations on  $H_s(N)$  (and *vice versa*). Thus, the remaining problem is to know the asymptotic behaviour of  $\pi_{N,k}$ , for  $N\to\infty$  [11]. For that, in this work, we are interested in the *combinatorial* aspects of these sums by use of a symbolic encoding by words. This enables then to transfer *shuffle relations* on words into algebraic relations between multiple harmonic sums, or between *polylogarithm* functions, defined for a multi-index  $\mathbf{s}=(s_1,\ldots,s_r)$  by

$$\operatorname{Li}_{\mathbf{s}}(z) = \sum_{n_1 > \dots > n_r > 0} \frac{z^{n_1}}{n_1^{s_1} \dots n_r^{s_r}}, \quad \text{for} \quad |z| < 1.$$
 (6)

These relations are recalled in Section 2. The reason to call upon polylogarithms is given in Section 3, since the generating function  $P_{\mathbf{s}}(z) = \sum_{n>0} H_{\mathbf{s}}(n) z^n$  of  $\{H_{\mathbf{s}}(n)\}_{n\geq 0}$ , verifies

$$P_{\mathbf{s}}(z) = \frac{1}{1-z} \operatorname{Li}_{\mathbf{s}}(z). \tag{7}$$

So, we set the polylogarithmic algebra of  $\{P_s\}_s$ , with coefficients in  $\mathcal{C}=\mathbb{C}[z,z^{-1},(z-1)^{-1}]$ , and we then establish *exact* transfer results between a function g in this algebra and its Taylor coefficients  $[z^N]g(z)$ , in the  $\mathbb{C}$ -algebra generated by  $\{N^k \operatorname{H}_s(N)\}_{s,\ k\in\mathbb{Z}}$  in both directions. The main result of this paper is finally stated in Section 4, which gives a computation of the *full* singular expansion of g, in the basis of functions  $\{(1-z)^{\alpha}\log^{\beta}(1-z)\}_{\alpha\in\mathbb{Z},\beta\in\mathbb{N}}$ , near the singularity z=1. We deduce from this a *full* asymptotic expansion of its Taylor coefficients. These results are based on the analysis of the *noncommutative* generating series of functions of the form (7), in particular on its infinite factorization indexed by *Lyndon words*.

## 2 Background

## 2.1 Combinatorics on words

To the multi-index s we can canonically associate the word  $u=x_0^{s_1-1}x_1\dots x_0^{s_r-1}x_1$  over the finite alphabet  $X=\{x_0,x_1\}$ . In the same way, s can be canonically associated to the word  $v=y_{s_1}\dots y_{s_r}$  over the infinite alphabet  $Y=\{y_i\}_{i\geq 1}$ . Moreover, in both alphabets, the empty multi-index will correspond to the empty word  $\epsilon$ . We shall henceforth identify the multi-index s with its encoding by the word u (resp. v). We denote by  $X^*$  (resp.  $Y^*$ ) the free monoid generated by X (resp. Y), which is the set of words over X (resp. Y). Noting  $\mathbb{C}\langle X\rangle$  (resp.  $\mathbb{C}\langle Y\rangle$ ) the algebra of noncommutative polynomials with coefficients in  $\mathbb{C}$ , we obtain so a concatenation isomorphism from the  $\mathbb{C}$ -algebra of multi-indexes into the algebra  $\mathbb{C}\langle X\rangle$  (resp.  $\mathbb{C}\langle Y\rangle$ ). The coefficient of  $w\in X^*$  in a polynomial  $S\in \mathbb{C}\langle X\rangle$  is denoted by (S|w) or  $S_w$ . The duality between polynomials is defined as follows

$$(S|p) = \sum_{w \in X^*} S_w p_w, \ p \in \mathbb{C}\langle X \rangle.$$
 (8)

The set of Lie monomials is defined by induction: the letters in X are Lie monomials and the Lie bracket [a,b]=ab-ba of two Lie monomials a and b is a Lie monomial. A Lie polynomial is a  $\mathbb{C}$ -linear combination of Lie monomials. The set of Lie polynomials is called the *free Lie algebra*.

#### 2.2 Shuffle products

Let  $a, b \in X$  (resp.  $y_i, y_j \in Y$ ) and  $u, v \in X^*$  (resp.  $Y^*$ ). The *shuffle* (resp. *stuffle*) of u = au' and v = bv' (resp.  $u = y_i u'$  and  $v = y_i v'$ ) is the polynomial recursively defined by

$$\epsilon \sqcup u = u \sqcup \epsilon = u \quad \text{and} \quad u \sqcup v = a(u' \sqcup v) + b(u \sqcup v'),$$
 (9)

(resp. 
$$\epsilon \sqcup u = u \sqcup \epsilon = u$$
 and  $u \sqcup v = y_i(u' \sqcup v) + y_i(u \sqcup v') + y_{i+j}(u' \sqcup v')$ ). (10)

#### Example 2.

$$x_0 x_1 \sqcup x_1 = x_1 x_0 x_1 + 2x_0 x_1^2 y_2 \sqcup y_1 = y_1 y_2 + y_2 y_1 + y_3.$$
 (11)

This product is extended to  $\mathbb{C}\langle X\rangle$  (resp.  $\mathbb{C}\langle Y\rangle$ ) by linearity. With this product,  $\mathbb{C}\langle X\rangle$  (resp.  $\mathbb{C}\langle Y\rangle$ ) is a commutative and associative  $\mathbb{C}$ -algebra.

l	$Q_l$	$\mathcal{S}_l$
$x_0$	$x_0$	$x_0$
$x_1$	$ x_1 $	$ x_1 $
$x_0x_1$	$[x_0, x_1]$	$x_0x_1$
$x_0^2 x_1$	$[x_0, [x_0, x_1]]$	$ x_0^2x_1 $
$x_0x_1^2$	$[[x_0, x_1], x_1]$	$ x_0x_1^2 $
$x_0^3 x_1$	$[x_0, [x_0, [x_0, x_1]]]$	$x_0^3 x_1$
:	<b>:</b>	<b>:</b>
$x_0^3 x_1^3$	$[x_0, [x_0, [[[x_0, x_1], x_1], x_1]]]$	$x_0^3 x_1^3$
$x_0^2 x_1 x_0 x_1^2$	$[x_0, [[x_0, x_1], [[x_0, x_1], x_1]]]$	$3x_0^3x_1^3 + x_0^2x_1x_0x_1^2$
$x_0^2 x_1^2 x_0 x_1$	$[[x_0, [[x_0, x_1], x_1]], [x_0, x_1]]$	$\left  6x_0^3x_1^3 + 3x_0^2x_1x_0x_1^2 + x_0^2x_1^2x_0x_1 \right $
$x_0^2 x_1^4$	$[x_0, [[[[x_0, x_1], x_1], x_1], x_1]]$	$ x_0^2x_1^4 $
$x_0x_1x_0x_1^3$	$ [[x_0, x_1], [[[x_0, x_1], x_1], x_1] $	
$x_0x_1^{5}$	$ [[[[[x_0, x_1], x_1], x_1], x_1], x_1] $	$x_0x_1^{5}$

Tab. 1: Lyndon words, bracket forms and dual basis

### 2.3 Lyndon words and Radford's theorem

By definition, a *Lyndon word* is a non empty word  $l \in X^*$  (resp.  $\in Y^*$ ) which is lower than any of its proper right factors [14] (for the lexicographical ordering) i.e. for all  $u, v \in X^* \setminus \{\epsilon\}$  (resp.  $\in Y^* \setminus \{\epsilon\}$ ),  $l = uv \Rightarrow l < v$ . The set of Lyndon words of X (resp. Y) is denoted by  $\mathcal{L}yn(X)$  (resp.  $\mathcal{L}yn(Y)$ ).

**Example 3.** For  $X = \{x_0, x_1\}$  with the order  $x_0 < x_1$  the Lyndon words of length  $\leq 5$  on  $X^*$  are (in lexicographical increasing order)

$$\{x_0, x_0^4x_1, x_0^3x_1, x_0^3x_1^2, x_0^2x_1, x_0^2x_1x_0x_1, x_0^2x_1^2, x_0^2x_1^3, x_0x_1, x_0x_1x_0x_1^2, x_0x_1^2, x_0x_1^3, x_0x_1^4, x_1\}.$$

For  $Y = \{y_i, i \geq 1\}$ , with the order  $y_i < y_j$  when i > j, here are the corresponding Lyndon words over Y

$$\{y_5, y_4, y_4y_1, y_3, y_3y_2, y_3y_1, y_3y_1^2, y_2, y_2^2y_1, y_2y_1, y_2y_1^2, y_2y_1^3, y_1\}.$$

Theorem 1 (Radford, [13, 14]). Let

$$C_1 = \mathbb{C} \oplus (\mathbb{C}\langle X \rangle \setminus x_0 \mathbb{C}\langle X \rangle x_1)$$
 and  $C_2 = \mathbb{C} \oplus (\mathbb{C}\langle Y \rangle \setminus y_1 \mathbb{C}\langle Y \rangle)$ 

be the sets of convergent polynomials over X and Y respectively. Then,

$$(\mathbb{C}\langle X\rangle, \sqcup) \simeq (\mathbb{C}[\mathcal{L}yn(X)], \sqcup) = (C_1[x_0, x_1], \sqcup),$$
  
$$(\mathbb{C}\langle Y\rangle, \sqcup) \simeq (\mathbb{C}[\mathcal{L}yn(Y)], \sqcup) = (C_2[y_1], \sqcup).$$

#### Example 4.

$$\begin{array}{rcl} y_2y_4y_1 + y_2y_1y_4 + y_1y_2y_4 + y_2y_5 + y_3y_4 & = & y_4 \mathrel{\sqcup}\!\!\sqcup y_2 \mathrel{\sqcup}\!\!\sqcup y_1 - y_4y_2 \mathrel{\sqcup}\!\!\sqcup y_1 - y_6 \mathrel{\sqcup}\!\!\sqcup y_1 \in \mathbb{C}[\mathcal{L}yn(Y)] \\ & = & y_2y_4 \mathrel{\sqcup}\!\!\sqcup y_1 \in \mathbb{C}_2[y_1] \end{array}$$

#### 2.4 Bracket forms and the dual basis

The bracket form  $Q_l$  of a Lyndon word l = uv, with  $l, u, v \in \mathcal{L}yn(X)$  and the word v being as long as possible, is defined recursively by

$$\begin{cases} \mathcal{Q}_l &= [\mathcal{Q}_u, \mathcal{Q}_v] \\ \mathcal{Q}_x &= x \text{ for each letter } x \in X, \end{cases}$$

It is classical that the set  $\mathcal{B}_1 = \{\mathcal{Q}_l : l \in \mathcal{L}yn(X)\}$ , ordered lexicographically, is a basis for the free Lie algebra. Moreover, each word  $w \in X^*$  can be expressed uniquely as a decreasing product of Lyndon words:

$$w = l_1^{\alpha_1} l_2^{\alpha_2} \dots l_k^{\alpha_k}, \quad l_1 > l_2 > \dots > l_k, \quad k \ge 0.$$
 (12)

The Poincaré–Birkhoff–Witt basis  $\mathcal{B} = \{\mathcal{Q}_w; w \in X^*\}$  and its dual basis  $\mathcal{B}^* = \{\mathcal{S}_w; w \in X^*\}$  are obtained from (12) by setting [14]

$$\begin{cases} \mathcal{Q}_w &= \mathcal{Q}_{l_1}^{\alpha_1} \mathcal{Q}_{l_2}^{\alpha_2} \dots \mathcal{Q}_{l_k}^{\alpha_k}, \\ \mathcal{S}_w &= \frac{\mathcal{S}_{l_1}^{\sqcup \sqcup \alpha_1} \sqcup \sqcup \ldots \sqcup \mathcal{S}_{l_k}^{\sqcup \sqcup \alpha_k}}{\alpha_1! \alpha_2! \ldots \alpha_k!}, \\ \mathcal{S}_l &= x \mathcal{S}_w, \quad \forall l \in \mathcal{L}yn(X), \text{ where } l = xw, \, x \in X, \, w \in X^*. \end{cases}$$

In [14], it is proved that  $\mathcal{B}$  and  $\mathcal{B}^*$  are dual bases of  $\mathbb{C}\langle X\rangle$  i.e.  $(\mathcal{Q}_u|\mathcal{S}_v)=\delta_u^v$ , for all words  $u,v\in X^*$  with  $\delta_u^v=1$  if u=v, otherwise 0.

**Lemma 1.** For all  $w \in x_0 X^* x_1$ , one has  $S_w \in x_0 \mathbb{Z}\langle X \rangle x_1$ .

*Proof.* The Lyndon words involved in the decomposition (12) of a word  $w \in X^*x_1$  (resp.  $w \in x_0X^*x_1$ ) all belong to  $X^*x_1$  (resp.  $x_0X^*x_1$ ).

## 2.5 Polylogarithms

Let  $\mathcal{C} = \mathbb{C}[z, 1/z, 1/(z-1)]$  and let  $\omega_0$  and  $\omega_1$  be the two following differential forms

$$\omega_0(z) = \frac{dz}{z}$$
 and  $\omega_1(z) = \frac{dz}{1-z}$ . (13)

One verifies the polylogarithm  $\mathrm{Li}_{\mathbf{s}}(z)$ , defined by Formula (6), is also the following *iterated integral* with respect to  $\omega_0$  and  $\omega_1$ 

$$\operatorname{Li}_{\mathbf{s}}(z) = \int_{0 \to z} \omega_0^{s_1 - 1} \omega_1 \cdots \omega_0^{s_r - 1} \omega_1. \tag{14}$$

Thanks to the bijection from  $Y^*$  to  $X^*x_1$  previously explained, we can index the polylogarithms by the words of  $X^*x_1$ , or indistinctly by the words of  $Y^*$ . We can extend (14) over  $X^*$  by putting

$$\operatorname{Li}_{\epsilon}(z) = 1$$
,  $\operatorname{Li}_{x_0}(z) = \log z$ ,  $\operatorname{Li}_{x_i w}(z) = \int_{0 \leadsto z} \omega_i(t) \operatorname{Li}_w(t)$ , for  $x_i \in X, w \in X^*$ . (15)

Therefore,  $Li_w$  verifies the following identity [4]

$$\forall u, v \in X^*, \quad \operatorname{Li}_{u + 1 + v} = \operatorname{Li}_u \operatorname{Li}_v.$$
 (16)

The extended definition enables to construct the noncommutative generating series [4]

$$L = \sum_{w \in X^*} \operatorname{Li}_w w \tag{17}$$

as being the unique solution of the *Drinfel'd equation*, i.e. the differential equation [4]

$$d\mathbf{L} = [x_0\omega_0 + x_1\omega_1]\mathbf{L},\tag{18}$$

satisfying the boundary condition

$$L(\varepsilon) = e^{x_0 \log \varepsilon} + o(\sqrt{\varepsilon}), \text{ when } \varepsilon \to 0^+.$$
 (19)

**Proposition 1** ([5]). Let  $\sigma$  be the monoid morphism defined over  $X^*$  by  $\sigma(x_0) = -x_1$  and  $\sigma(x_1) = -x_0$ . Then,

$$L(1-z) = [\sigma L(z)] \prod_{l \in \mathcal{L}yn(X) \setminus \{x_0, x_1\}} e^{\zeta(S_l)Q_l}.$$

**Example 5 ([5]).** 

#### 2.6 Harmonic sums

**Definition 1.** Let  $w = y_{s_1} \dots y_{s_r} \in Y^*$ . For  $N \ge r \ge 1$ , the harmonic sum  $H_w(N)$  is defined as

$$H_w(N) = \sum_{N \ge n_1 > \dots > n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}}.$$

For  $0 \le N < r$ ,  $H_w(N) = 0$  and, for the empty word  $\epsilon$ , we put  $H_{\epsilon}(N) = 1$ , for any  $N \ge 0$ .

Let  $w = y_{s_1} \dots y_{s_r} \in Y^*$ . If  $s_1 > 1$  then, by an Abel's theorem,

$$\lim_{N \to \infty} H_w(N) = \lim_{z \to 1} \text{Li}_w(z) = \sum_{n_1 > \dots > n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}}.$$

That is nothing but the polyzêta (or MZV [16])  $\zeta(w)$  and the word  $w \in Y^* \setminus y_1 Y^*$  is said to be *convergent*. A polynomial of  $\mathbb{C}\langle Y \rangle$  is said to be convergent when it is a linear combination of convergent words. The *double* shuffle algebra of polyzêtas is already pointed out and extensively studied in [3].

For  $w = y_s w'$ , we have

$$\zeta(w) = \sum_{l>1} \frac{H_{w'}(l-1)}{l^s},$$
 (20)

$$H_w(N+1) - H_w(N) = (N+1)^{-s} H_{w'}(N)$$
 (21)

and, for any  $u, v \in Y^*$  [9]

$$H_{u \perp v}(N) = H_{u}(N)H_{v}(N). \tag{22}$$

## 3 Generating series

## 3.1 Definition and first properties

**Definition 2** ([8]). Let  $w \in Y^*$  and let  $P_w(z)$  be the ordinary generating series of  $\{H_w(N)\}_{N\geq 0}$ 

$$P_w(z) = \sum_{N>0} H_w(N) z^N.$$

**Proposition 2 ([8]).** Extended by linearity, the map  $P: u \mapsto P_u$  is an isomorphism from  $(\mathbb{C}\langle Y \rangle, \bowtie)$  to the Hadamard algebra of  $(\{P_w\}_{w \in Y^*}, \odot)$ . Therefore, the map  $H: u \mapsto H_u = \{H_u(N)\}_{N \geq 0}$  is an isomorphism from  $(\mathbb{C}\langle Y \rangle, \bowtie)$  to the algebra of  $(\{H_w\}_{w \in Y^*}, .)$ .

*Proof.* The definition of the Hadamard product  $\sum_{n=0}^{\infty} a_n z^n \odot \sum_{n=0}^{\infty} b_n z^n = \sum_{n=0}^{\infty} a_n b_n z^n$ , and the formula (22) gives P as an algebra morphism. Since the functions  $\{\operatorname{Li}_w\}_{w\in X^*}$  are linearly independent over  $\mathcal{C}$  [4], P is the expected isomorphism.

**Proposition 3 ([8]).** For every word  $w \in Y^*$  and for  $z \in \mathbb{C}$  satisfying |z| < 1, one has  $\mathrm{Li}_w(z) = (1-z)\mathrm{P}_w(z)$ .

*Proof.* For  $w = y_s w'$ , since  $P_w(z) = \sum_{N>0} H_w(N) z^N$  and by using (21),

$$(1-z)P_w(z) = H_w(0) + \sum_{N>1} \frac{H_{w'}(N-1)}{N^s} z^N = \text{Li}_w(z).$$

A direct consequence of this proposition and Identity (16) is

**Corollary 1.** For all  $u, v \in X^*$ , for all  $z \in \mathbb{C}$  satisfying |z| < 1,  $P_u(z)P_v(z) = (1-z)^{-1}P_{u \sqcup v}(z)$ .

**Example 6.** Since  $x_1 = x_1 x_0 x_1 = x_1 x_0 x_1 + 2x_0 x_1^2$  then we get

$$P_{1,2}(z) = (1-z)P_1(z)P_2(z) - 2P_{2,1}(z).$$

Proposition 3 allows to extend the definition of  $P_w$  over  $X^*$  as we have already extended the definition of  $\operatorname{Li}_w$  over  $X^*$ . Moreover,

**Definition 3** ([8]). Let P be the noncommutative generating series of  $\{P_w\}_{w \in X^*}$ :

$$P = \sum_{w \in X^*} P_w w.$$

**Proposition 4 ([8]).** Let  $\sigma$  be the monoid morphism defined over  $X^*$  by  $\sigma(x_0) = -x_1$  and  $\sigma(x_1) = -x_0$ . Then

$$P(1-z) = \frac{1-z}{z} [\sigma P(z)] \prod_{l \in \mathcal{L}yn(X) \setminus \{x_0, x_1\}}^{\searrow} e^{\zeta(S_l)Q_l}.$$

*Proof.* It follows immediately from Proposition 1.

#### Example 7.

$$P_{2,1}(1-z) = \frac{1-z}{z} \left( -P_3(z) + \log(z)P_2(z) - \log^2(z)P_1(z) + \frac{\zeta(3)}{1-z} \right)$$

Thus,

$$P_{2,1}(z) = -\frac{z}{1-z}P_3(1-z) + \frac{z\log(1-z)}{1-z}P_2(1-z) - \frac{1}{2}\frac{z\log^2(1-z)}{1-z}P_1(1-z) + \frac{\zeta(3)}{1-z}.$$

By Formula (22) and Proposition 2, for  $w \in Y^*$ , there exist a finite set I and  $(c_i)_{i \in I} \in \mathcal{C}_2^I$  such that the three following identities are equivalent

$$w = \sum_{i \in I} c_i \bowtie y_1^{\bowtie i}, \tag{23}$$

$$P_w = \sum_{i \in I} P_{c_i} \odot P_{y_1}^{\odot i}, \tag{24}$$

$$\mathbf{H}_w = \sum_{i \in I} \mathbf{H}_{c_i} \, \mathbf{H}_{y_1}^i. \tag{25}$$

In particular, for  $w = y_1^k$ , we have,

**Lemma 2.** Let  $M = (m_{i,j})_{1 \le i,j \le k}$  be the matrix defined by  $m_{i,j} = \delta_{i,j+1}$  (Kronecker symbol). Let  $e_{i,j}$  the matrix of size  $k \times k$ , whose coefficients are all zero, except the one equal to 1 at line i and column j. Let

$$A = \begin{pmatrix} y_1 & 0 & \dots & 0 \\ -\frac{y_2}{2} & \frac{y_1}{2} & \dots & 0 \\ \vdots & \ddots & \ddots & 0 \\ \frac{(-1)^{k-1}y_k}{k} & \frac{(-1)^{k-2}y_{k-1}}{k} & \dots & \frac{y_1}{k} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} H_{y_1} & 0 & \dots & 0 \\ -\frac{H_{y_2}}{2} & \frac{H_{y_1}}{2} & \dots & 0 \\ \vdots & \ddots & \ddots & 0 \\ \frac{(-1)^{k-1}H_{y_k}}{k} & \frac{(-1)^{k-2}H_{y_{k-1}}}{k} & \dots & \frac{H_{y_1}}{k} \end{pmatrix}.$$

Then

$$\begin{pmatrix} y_1 \\ \vdots \\ y_1^k \end{pmatrix} = A \prod_{\ell=1}^{k-1} \left[ M^\ell A(^t M)^\ell + \sum_{\iota=1}^\ell e_{\iota,\iota} \right] \begin{pmatrix} \epsilon \\ \vdots \\ \epsilon \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathcal{H}_{y_1} \\ \vdots \\ \mathcal{H}_{y_1^k} \end{pmatrix} = B \prod_{\ell=1}^{k-1} \left[ M^\ell B(^t M)^\ell + \sum_{\iota=1}^\ell e_{\iota,\iota} \right] \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$$

*Proof.* The formula  $y_1^k = (-1)^{k-1}k^{-1}\sum_{l=0}^{k-1}(-1)^ly_1^l \bowtie y_{k-l}$  [6] can be written matricially as follows

$$\begin{pmatrix} y_1 \\ y_1^2 \\ \vdots \\ y_1^k \end{pmatrix} = A \bowtie \begin{pmatrix} \epsilon \\ y_1 \\ \vdots \\ y_1^{k-1} \end{pmatrix} = A \bowtie \begin{pmatrix} \epsilon & 0 & \dots & 0 \\ 0 & y_1 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & \frac{(-1)^{k-2}y_{k-1}}{k-1} & \dots & \frac{y_1}{k-1} \end{pmatrix} \bowtie \begin{pmatrix} \epsilon \\ \epsilon \\ \vdots \\ y_1^{k-2} \end{pmatrix}.$$

Here all powers and products are carried out with the stuffle product. Successively, we get the expected result.  $\Box$ 

The word  $y_1^k$  appears then as a computable stuffle product of words of length 1. Hence,

**Proposition 5.**  $H_{y_k^k}$  is a combination of  $\{H_{y_r}\}_{1 \le r < k}$  which are algebraically independent.

*Proof.* The  $\{H_{y_r}\}_{1 \le r < k}$  are algebraically independent according to Proposition 2, as image by the isomorphism H of the Lyndon words  $\{y_r\}_{1 \le r < k}$ . By Lemma 2, we get the expected result.

#### Example 8. Since

$$y_1^2 = \frac{y_1 \coprod y_1 - y_2}{2}$$
 and  $y_1^3 = \frac{2(y_3 - y_1 \coprod y_2) + (y_1 \coprod y_1 - y_2) \coprod y_1}{6}$ 

then we have

$$\mathbf{H}_{y_1^2} = \frac{\mathbf{H}_{y_1}^2 - \mathbf{H}_{y_2}}{2} \quad \textit{and} \quad \mathbf{H}_{y_1^3} = \frac{2(\mathbf{H}_{y_3} - \mathbf{H}_{y_1}\mathbf{H}_{y_2}) + (\mathbf{H}_{y_1}^2 - \mathbf{H}_{y_2})\mathbf{H}_{y_1}}{6}.$$

Identities (23-25) give rise to two interpretations: (24) enables to decompose  $P_w$  in a basis of singular functions  $(1-z)^{\alpha}\log^{\beta}(1-z)$  while (25) enables to compute an asymptotic expansion of its Taylor coefficients in terms of  $N^a\log^b N$  (or equivalently in terms of  $N^aH^b_{y_1}(N)$ ). Before stating a theorem linking these two interpretations, we are interested in the action of  $\mathcal C$  on Taylor coefficients; reciprocally, we are interested in the effects of changing Taylor coefficients on a function in  $\mathcal C[\{P_w\}_{w\in Y^*}]$ .

## 3.2 Operations on the generating functions $P_w$

For  $f(z) = \sum_{n \geq 0} a_n z^n$ , we will henceforth denote  $[z^n] f(z) = a_n$  its *n*-th Taylor coefficient. Since multiplying or dividing by z acts very simply on  $[z^n] f(z)$ , we only have to study the effect of multiplying or dividing by 1 - z.

$$[z^n](1-z)P_w(z) = H_w(n) - H_w(n-1).$$
(26)

$$[z^n] \frac{P_w(z)}{1-z} = \sum_{k=0}^n H_w(k)$$
 (27)

$$=\begin{cases} (n+1)H_w(n) - H_{y_{s-1}w'}(n) & \text{if } w = y_sw', \text{ with } s \neq 1\\ (n+1)H_w(n) - \sum_{j=1}^n H_{w'}(j-1) & \text{if } w = y_1w'. \end{cases}$$
(28)

and, more generally,

#### Proposition 6.

$$[z^n](1-z)^k P_w(z) = \sum_{j=0}^k \binom{k}{j} (-1)^j H_w(n-j) \quad \text{and} \quad [z^n] \frac{P_w(z)}{(1-z)^k} = \sum_{n \geq j_1 > \dots > j_k \geq 0} H_w(j_k).$$

### 3.3 Operations on Taylor coefficients of $P_w$

We are now to find how multiplying or dividing  $H_w(N)$  by N acts on  $P_w$ .

#### 3.3.1 A particular case : $w = \epsilon$

The simple case  $w = \epsilon$ , corresponding to  $H_{\epsilon}(N) = 1$ , can be studied and treated by the following

**Proposition 7.** For any  $q \in \mathbb{Z}$ , one has

$$n^{q} = \begin{cases} [z^{n}](1-z)P_{-q}(z) & \text{if } q < 0, \\ [z^{n}](1-z)^{-1} & \text{if } q = 0, \\ [z^{n}]\frac{z}{1-z}N_{q}\left(\frac{1}{1-z}\right) & \text{if } q > 0, \end{cases}$$

where  $N_q$  is defined by the following recurrence

$$N_0(X) = 1$$
, and  $N_q(X) = X \left( \sum_{j=0}^{q-1} (-1)^{q-1-j} \binom{q}{j} N_j(X) \right)$ .

#### Example 9.

$$n = [z^n] \left( \frac{z}{(1-z)^2} \right) = [z^n] \left( \frac{1}{(1-z)^2} - \frac{1}{1-z} \right),$$

$$n^2 = [z^n] \left( \frac{2z}{(1-z)^3} - \frac{z}{(1-z)^2} \right) = [z^n] \left( \frac{2}{(1-z)^3} - \frac{3}{(1-z)^2} + \frac{1}{1-z} \right).$$

## 3.3.2 How to divide by $n^k$ ?

Let  $w = y_{s_1} \cdots y_{s_r}$  and  $w' = y_{s_2} \cdots y_{s_r}$  be the suffix of w, of length r-1. The expression  $n^{-k}H_w(n)$ , k positive integer, can be identified as follows

$$n^{-k}H_w(n) = n^{-k}H_w(n-1) + n^{-s_1-k}H_{w'}(n-1)$$
(29)

$$= [z^n] \operatorname{Li}_{y_k w + y_{s_1 + k} w'}(z) \tag{30}$$

$$= [z^n][(1-z)P_{y_kw+y_{s_1+k}w'}(z)].$$
(31)

## 3.3.3 How to multiply by $n^k$ ?

In order to study the effect of multiplying by  $n^k$ , k positive integer, we denote by  $\theta = z\partial/\partial z$  the Euler operator. Then for any integer k,

$$n^k \mathbf{H}_w(n) = [z^n] \theta^k \mathbf{P}_w(z). \tag{32}$$

So, we just have to compute  $\theta^k P_w(z)$ . As in [7], let us introduce

**Definition 4.** For any word  $w = x_{i_1} \cdots x_{i_k}$  and for any composition  $\mathbf{r} = (r_1, \dots, r_k)$ , let  $\tau_{\mathbf{r}}(w)$  be defined by  $\tau_{\mathbf{r}}(w) = \tau_{r_1}(x_{i_1}) \cdots \tau_{r_k}(x_{i_k})$  with,

$$au_0(x_0) = x_0\,, \qquad au_r(x_1) = x_1, \\ and, \ for \ r \in \mathbb{N}^*, \quad au_r(x_0) = heta^r x_0 = 0 \quad and \quad au_r(x_1) = heta^r rac{zx_1}{1-z} = rac{r!x_1}{(1-z)^{r+1}}.$$

We define the degree of  $\mathbf{r}$  by  $\deg(\mathbf{r}) = k$  and its weight by  $\operatorname{wgt}(\mathbf{r}) = k + r_1 + \cdots + r_k$ .

By applying successively the operator  $\theta$  to L, we get

**Lemma 3.**  $\theta^l L = A_l L$ , where  $A_l$  is defined by

$$A_l(z) = \sum_{\text{wgt}(\mathbf{r}) = l} \sum_{w \in X^{\text{deg}(\mathbf{r})}} \prod_{i=1}^{\text{deg}(\mathbf{r})} {\binom{\sum_{j=1}^i r_i + j - 1}{r_i}} \tau_{\mathbf{r}}(w).$$

*Proof.* This is a consequence of the recurrence relation verified by  $A_l$ , which is  $A_0(z)=1$ , and, for all  $l\in\mathbb{N}, A_{l+1}(z)=[\tau_0(x_0)+\tau_0(x_1)]A_l(z)+\theta A_l(z).$ 

This lemma enables to extract the expression of  $\theta^l \operatorname{Li}_w$ , for any word  $w \in X^*$ .

#### Example 10.

$$A_0(z) = 1,$$

$$A_1(z) = x_0 + \frac{z}{1-z}x_1,$$

$$A_2(z) = x_0^2 + \frac{z}{1-z}x_0 \sqcup x_1 + \frac{z^2}{(1-z)^2}x_1^2 + \frac{1}{(1-z)^2}x_1.$$

So, for  $w = x_0^2 x_1$ ,

$$\begin{split} \theta \operatorname{Li}_{x_0^2 x_1} &= \left( (x_0 + \frac{z}{1-z} x_1) \operatorname{L}(z) \mid x_0^2 x_1 \right) \\ &= \operatorname{Li}_{x_0 x_1}, \\ \theta^2 \operatorname{Li}_{x_0^2 x_1} &= \left( (x_0^2 + \frac{z}{1-z} x_0 \sqcup x_1 + \frac{z^2}{(1-z)^2} x_1^2 + \frac{1}{(1-z)^2} x_1) \operatorname{L}(z) \mid x_0^2 x_1 \right) \\ &= \operatorname{Li}_{x_1}. \end{split}$$

**Lemma 4.** Let  $\bot$  be the linear operator of  $\mathbb{Z}[X]$  defined by  $\bot X^n = (n+1)X^{n+1} + nX^n$  and  $\{B_l\}_{l \in \mathbb{N}} \in \mathbb{Z}[X]$  defined by  $B_0(X) = 1$  and  $B_{l+1}(X) = \bot B_l(X)$ . Then

$$\theta^{l}(1-z)^{-1} = (1-z)^{-1}B_{l}(z(1-z)^{-1}).$$

Note that the head term of  $B_l$ ,  $l \ge 1$ , is  $l!X^l$  and its trail term is X.

**Example 11.**  $B_0(X) = 1$ ,  $B_1(X) = X$ ,  $B_2(X) = 2X^2 + X$ ,  $B_3(X) = 6X^3 + 6X^2 + X$ .

**Proposition 8.** With the notations of Lemma 4,

$$\theta^k P(z) = \sum_{j=1}^k \sum_{\text{wgt}(\mathbf{r})} \sum_{w \in X^{\text{deg}(\mathbf{r})}} \prod_{i=1}^{\text{deg}(\mathbf{r})} {\sum_{j=1}^i r_i + j - 1 \choose r_i} {\binom{k}{j}} \tau_{\mathbf{r}}(w) B_j \left(\frac{z}{1-z}\right) P(z).$$

Using Leibniz formula, one has

$$\theta^k \mathcal{P}_w(z) = \sum_{j=0}^k \binom{k}{j} \theta^{k-j} \operatorname{Li}_w(z) \theta^j \frac{1}{1-z}$$
(33)

$$= \sum_{j=0}^{k} {k \choose j} B_j \left(\frac{z}{1-z}\right) \frac{1}{1-z} \theta^{k-j} \operatorname{Li}_w(z). \tag{34}$$

Thanks to Lemma 3, we can extract the coefficient  $\theta^l \operatorname{Li}_w$  of w in  $\theta^l \operatorname{L}$ : this can be written as  $\mathcal{C}$ -linear combination of  $\operatorname{Li}_v$ , with  $|v| \leq |w| - l$  (where |u| denotes the length of a word  $u \in X^*$ ). We deduce so the expression of  $\theta^k \operatorname{P}_w$ .

**Example 12.** For  $w = x_0^2 x_1$  and k = 2,

$$\begin{split} \theta^2 \mathbf{P}_{x_0^2 x_1}(z) &= \sum_{j=0}^2 \binom{2}{j} B_j \left(\frac{z}{1-z}\right) \frac{1}{1-z} \theta^{2-j} \operatorname{Li}_w(z) \\ &= \frac{1}{1-z} \operatorname{Li}_{x_1}(z) + 2 \frac{z}{1-z} \frac{1}{1-z} \operatorname{Li}_{x_0 x_1}(z) + \left(2 \left(\frac{z}{1-z}\right)^2 + \frac{z}{1-z}\right) \operatorname{Li}_{x_0^2 x_1}(z) \\ &= \mathbf{P}_{x_1}(z) + \frac{2z}{1-z} \mathbf{P}_{x_0 x_1}(z) + \frac{z^2+z}{1-z} \mathbf{P}_{x_0^2 x_1}(z). \end{split}$$
 So, 
$$n^2 \mathbf{H}_3(n) &= [z^n] \left(\mathbf{P}_1(z) + \frac{2z}{1-z} \mathbf{P}_2(z) + \frac{z^2+z}{1-z} \mathbf{P}_3(z)\right).$$

#### 4 The main theorem

Throughout the section, we will write

$$f_n \sim \sum_{i=0}^{\infty} g_i(n)$$
 for  $n \to +\infty$ ,

for a scale of functions  $(g_i)_{i\in\mathbb{N}}$  – i.e. verifying  $g_{i+1}(n) = O(g_i(n))$ , for all i – to express that

$$f_n = \sum_{i=0}^{I} g_i(n) + O(g_{I+1}(n)), \quad \text{for any } I \ge 0.$$

In the same way, given a scale of functions  $(h_i)_{i\in\mathbb{N}}$  around z=1 (i.e. verifying  $h_{i+1}(1-z)=O(h_i(1-z))$ , when  $z\to 1$ ) we will write

$$g(z) \sim \sum_{i=0}^{\infty} h_i (1-z)$$
 for  $z \to 1$ ,

to mean

$$g(z) = \sum_{i=0}^{I} h_i(1-z) + O(h_{I+1}(1-z))$$
 for all  $I \ge 0$ .

For  $w=y_1^k$ , we know the expression of  $[z^N]P_{y_1^k}(z)=H_{y_1^k}(N)$  is given by Lemma 2. From the second form of Euler-MacLaurin formula, involving the Bernoulli numbers  $\{B_k\}_{k\geq 0}$ , we get the following asymptotic expansions

$$\begin{split} & \mathbf{H}_{y_1}(N) & \sim & \log N + \gamma - \sum_{k=1}^{+\infty} \frac{B_k}{k} \frac{1}{N^k}, \\ & \mathbf{H}_{y_r}(N) & \sim & \zeta(r) - \frac{1}{(r-1)N^{r-1}} - \sum_{k=r}^{+\infty} \frac{B_{k-r+1}}{k-r+1} \binom{k-1}{r-1} \frac{1}{N^k}, \text{ for } r > 1. \end{split}$$

Thus, we can deduce the asymptotic expansions of  $H_{y_1^k}(N)$ , for  $N \to +\infty$ , from the asymptotic expansions of  $\{H_{y_r}(N)\}_{1 \le r \le k}$ :

Example 13. From Example 8, we can deduce then

$$\begin{split} \mathrm{H}_{y_1^2}(N) &= \frac{1}{2}(\log(N) + \gamma)^2 - \frac{1}{2}\zeta(2) + \frac{1}{2}\frac{\log(N) + \gamma + 1}{N} - \frac{1}{12N^2} + \mathrm{O}\left(\frac{1}{N^2}\right), \\ \mathrm{H}_{y_1^3}(N) &= \frac{1}{6}\log^3(N) + \frac{1}{2}\gamma\log^2(N) + \frac{1}{2}(\gamma^2 - \zeta(2))\log(N) - \frac{1}{2}\zeta(2)\gamma + \frac{1}{3}\zeta(3) + \frac{1}{6}\gamma^3 + \frac{1}{4}\frac{\log^2(N)}{N} \\ &+ \frac{1}{2}(\gamma + 1)\frac{\log(N)}{N} + \frac{1}{4}\left(2\gamma + \gamma^2 - \zeta(2)\right)\frac{1}{N} - \frac{1}{24}\frac{\log^2(N)}{N^2} - \left(\frac{1}{8} + \frac{\gamma}{12}\right)\frac{\log(N)}{N^2} + \mathrm{O}\left(\frac{1}{N^2}\right). \end{split}$$

Let us see in the general case how to reach the Taylor expansion of  $g \in \mathcal{C}[(P_w)_{w \in Y^*}]$ .

**Theorem 2.** Let  $g \in \mathcal{C}[(P_w)_{w \in Y^*}]$ . There exist  $a_j \in \mathbb{C}$ ,  $\alpha_j \in \mathbb{Z}$  and  $\beta_j \in \mathbb{N}$  such that

$$g(z) \sim \sum_{j=0}^{+\infty} a_j (1-z)^{\alpha_j} \log^{\beta_j} (1-z), \text{ for } z \to 1.$$

Therefore, there exist  $b_i \in \mathbb{C}$ ,  $\eta_i \in \mathbb{Z}$  and  $\kappa_i \in \mathbb{N}$  such that

$$[z^n]g(z) \sim \sum_{i=0}^{+\infty} b_i n^{\eta_i} \log^{\kappa_i}(n), \quad for \quad n \to \infty.$$

*Proof.* Considering Corollary 1, we only have firstly to obtain the asymptotic expansion for the case  $g(z) = P_w(z)$ . Indeed, we get then the expansions of f(z)g(z), for  $f \in \mathcal{C}$  by remarking that z = 1 - (1 - z) and that  $z^{-1} = \sum_{n \geq 0} (1 - z)^n$ .

The first expansion can be derived from Proposition 4 which links the behaviour of  $P_w$  around z=1 to the behaviour of some algebraic combination of functions  $\{P_u\}_{u\in X^*}$  around z=0. Moreover, by Radford theorem 1, we can assume that each word u involved in this combination is a Lyndon word and so belongs to  $x_0X^*x_1\cup\{x_0,x_1\}$ . But, remind that, in this case, we have  $P_u(z)=\sum_{n\geq 0}H_u(n)z^n$  and that  $P_{x_0}(z)=(1-z)^{-1}\log(z)$ . So, the expected first expansion follows.

From

$$(1-z)^{\alpha}\log(1-z)^{\beta} = (-1)^{\beta}\beta!(1-z)^{\alpha+1}P_{y_1^{\beta}}(z), \tag{35}$$

we derive the second expansion by computing the Taylor coefficient  $[z^n](1-z)^{\alpha}\log^{\beta}(1-z)$ . Since we have already explained how the multiplication by  $(1-z)^{\alpha}$  acts on the Taylor coefficients, we just have then to compute  $[z^n]P_{y_1^{\beta}}=H_{y_1^{\beta}}(n)$ . For this, we use Lemma 2 which completes our proof.

Unfortunately, in the general case, knowing even the complete expansion of  $[z^n]g(z)$  only enables to get an asymptotic expansion of g(z), as  $z \to 1$  up to order 0 (i.e. the *singular part* of the expansion). Indeed, Taylor coefficients of all functions  $(1-z)^k$ ,  $k \ge 0$  eventually vanish as in the following identity:

$$\frac{1}{n} = [z^n] \operatorname{Li}_1(z) = [z^n] [\operatorname{Li}_1(z) + (1-z)^2], \quad \text{as soon as } n > 2.$$
 (36)

In fact, to obtain this singular part, it is sufficient to know the asymptotic expansion of  $[z^n]g(z)$  up to order  $2 - \epsilon$ ,  $\epsilon > 0$  [15].

**Remark 1.** In the case of a finite sum  $\sum_{i \in I} b_i n^{\eta_i} H_1^{\kappa_i}(n)$ , we are able to construct the unique function  $f \in \mathcal{C}[(P_w)_{w \in Y^*}]$  such that,

$$\forall n \in \mathbb{N}, \qquad [z^n] f(z) = \sum_{i \in I} b_i n^{\eta_i} \mathcal{H}_1^{\kappa_i}(n), \tag{37}$$

as illustrated in Examples 9 and 12.

**Remark 2.** Note that the proof of Theorem 2 gives an effective construction of the asymptotic expansion of Taylor coefficients. In particular, applied to  $g(z) = P_w(z)$  directly, it enables to find an asymptotic expansion of  $H_w(N)$ , as shown in the corollary below. Another algorithm, based on Euler Mac-Laurin formula, is available in [1].

**Corollary 2.** Let  $\mathcal{Z}$  be the  $\mathbb{Q}$ -algebra generated by convergent polyzêtas and let  $\mathcal{Z}'$  be the  $\mathbb{Q}[\gamma]$ -algebra generated by  $\mathcal{Z}$ . Then there exist algorithmically computable coefficients  $b_i \in \mathcal{Z}'$ ,  $\kappa_i \in \mathbb{N}$  and  $\eta_i \in \mathbb{Z}$  such that, for any  $w \in Y^*$ ,

$$H_w(N) \sim \sum_{i=0}^{+\infty} b_i N^{\eta_i} \log^{\kappa_i}(N), \quad for \quad N \to +\infty.$$

**Example 14.** From Example 7 we get, for  $z \rightarrow 1$ 

$$P_{2,1}(z) = \frac{\zeta(3)}{1-z} + \log(1-z) - 1 - \frac{\log^2(1-z)}{2} + (1-z)\left(-\frac{\log^2(1-z)}{4} + \frac{\log(1-z)}{4}\right) + O(|1-z|).$$

But

$$\begin{split} [z^N]\zeta(3)(1-z)^{-1} &=& \zeta(3),\\ [z^N]\log(1-z) &=& -N^{-1},\\ [z^N]\frac{\log^2(1-z)}{2} &=& [z^N]\frac{2!(1-z)\mathrm{P}_{y_1^2}(z)}{2}\\ &=& [z^N](1-z)\mathrm{P}_{y_1^2}(z)\\ &=& \mathrm{H}_{y_1^2}(N)-\mathrm{H}_{y_1^2}(N-1),\\ \vdots &\vdots \end{split}$$

We find finally, using Example 13:

$$[z^N]P_{2,1}(z) = H_{2,1}(N) = \zeta(3) - \frac{\log(N) + 1 + \gamma}{N} + \frac{1}{2}\frac{\log(N)}{N^2} + O\left(\frac{1}{N^2}\right).$$

Otherwise, by Example 6,

$$\begin{array}{lcl} {\rm P}_{1,2}(z) & = & (1-z){\rm P}_1(z){\rm P}_2(z) - 2{\rm P}_{2,1}(z) \\ & = & (1-z)\frac{-\log(1-z)}{1-z}\frac{z}{1-z}\left(-{\rm P}_2(1-z) + \log(1-z){\rm P}_1(1-z) + \frac{\zeta(2)}{z}\right) - 2{\rm P}_{2,1}(z), \end{array}$$

calculated thanks to Proposition 4. So,

$$[z^N]P_{1,2}(z) = H_{1,2}(N) = \zeta(2)\gamma - 2\zeta(3) + \zeta(2)\log(N) + \frac{\zeta(2) + 2}{2N} + O\left(\frac{1}{N^2}\right).$$

**Corollary 3** ([8]). For any  $w \in Y^*$ , the N-free term in the asymptotic expansion of  $H_w(N)$ , when  $N \to +\infty$ , is a polynomial  $q_w$  in  $\mathbb{Z}[\gamma]$ . This term is an element in  $\mathbb{Z}$ , if and only if w is a convergent word.

**Example 15.** 
$$q_{y_1y_2} = \zeta(2)\gamma - 2\zeta(3)$$
 and  $q_{y_2y_1} = \zeta(3) = \zeta(2,1)$ .

**Question.** For any convergent word w, are  $\zeta(w)$  and  $\gamma$  algebraically independent?

Now, let us go back to the  $A_s$  introduced in Section 1. We have seen that they are  $\mathbb{Z}$ -linear combinations on  $H_s$ , hence we get their asymptotic expansions with coefficients in  $\mathbb{Z}'$ .

**Example 16.** For s = (1, 1, 1),

$$\begin{split} \mathbf{A}_{1,1,1}(N) &=& \ \mathbf{H}_{1,1,1}(N) + \mathbf{H}_{1,2}(N) + \mathbf{H}_{2,1}(N) + \mathbf{H}_{3}(N), \\ &=& \ \frac{1}{6} \log^3(N) + \frac{1}{2} \gamma \log^2(N) + \frac{1}{2} [\gamma^2 + \zeta(2)] \log(N) - \frac{1}{2} \zeta(2) \gamma + \frac{1}{3} \zeta(3) + \frac{1}{6} \gamma^3 + \frac{1}{4} \frac{\log^2(N)}{N} \\ &+& \ \frac{1}{2} (\gamma - 1) \frac{\log(N)}{N} + \frac{1}{4} [\gamma^2 - 2\gamma + \zeta(2)] \frac{1}{N} - \frac{1}{24} \frac{\log^2(N)}{N^2} + \frac{1}{24} (9 - 2\gamma) \frac{\log(N)}{N^2} + \mathcal{O}\left(\frac{1}{N^2}\right). \end{split}$$

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#### References

- [1] C. Costermans, J.Y. Enjalbert, Hoang Ngoc Minh, M. Petitot.— *Structure and asymptotic expansion of multiple harmonic sums*, in the proceeding of ISSAC, Beijing, 24-27 July, (2005).
- [2] P. Flajolet, G. Gonnet, C. Puech, and J. M. Robson. *Analytic variations on quadtrees*, Algorithmica, 10, pp. 473-500, 1993.
- [3] Hoang Ngoc Minh & M. Petitot.— Lyndon words, polylogarithmic functions and the Riemann  $\zeta$  function, Discrete Math., 217, 2000, pp. 273-292.
- [4] Hoang Ngoc Minh, M. Petitot & J. Van der Hoeven.— *Polylogarithms and Shuffle Algebra*, FP-SAC'98, Toronto, Canada, Juin 1998.
- [5] Hoang Ngoc Minh, M. Petitot & J. Van der Hoeven.— L'algèbre des polylogarithmes par les séries génératrices, FPSAC'99, Barcelone, Espagne, Juillet 1999.
- [6] Hoang Ngoc Minh, G. Jacob, N.E. Oussous, M. Petitot.— De l'algèbre des ζ de Riemann multivariées à l'algèbre des ζ de Hurwitz multivariées, journal électronique du Séminaire Lotharingien de Combinatoire B44e, 2001.
- [7] Hoang Ngoc Minh.— Differential Galois groups and noncommutative generating series of polylogarithms, in the proceeding of 7<sup>th</sup> World Multiconference on Systemics, Cybernetics and informatics, pp. 128-135, Orlando, Florida, July (2003).
- [8] Hoang Ngoc Minh.– Finite polyzêtas, Poly-Bernoulli numbers, identities of polyzêtas and noncommutative rational power series, in the proceeding of 4<sup>th</sup> International Conference on Words, pp. 232-250, Turku, Finland, September (2003)
- [9] M. Hoffman. The algebra of multiple harmonic series, Jour. of Alg., August 1997.
- [10] M. Hoffman.– *Hopf Algebras and Multiple Harmonic Sums*, Loops and Legs in Quantum Field Theory, Zinnowitz, Germany, April 2004.
- [11] G. Labelle. Communication privée, SFCA,96, Minneapolis.
- [12] L. Laforest.— *Etude des arbres hyperquaternaires*, Tech. Rep. 3, LACIM, UQAM, Montreal, Nov. 1990. (Ph.D. thesis, McGill University).
- [13] D.E. Radford.— A natural ring basis for shuffle algebra and an application to group schemes, Journal of Algebra, 58, pp. 432-454, 1979.
- [14] C. Reutenauer. Free Lie Algebras, Lon. Math. Soc. Mono., New Series-7, Oxford Science Publications, 1993.
- [15] M. Waldschmidt.— http://www.institut.math.jussieu.fr/~miw/articles/pdf/dea-juin2002.pdf, http://www.institut.math.jussieu.fr/~miw/articles/pdf/corrige-dea-juin2002.pdf
- [16] D. Zagier.— *Values of zeta functions and their applications*, First European congress of Mathematics, Vol.2, Birkhäuser, Basel, 1994, pp. 497-512.