Algorithmic and combinatoric aspects of multiple harmonic sums

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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 $\mathrm{H}_j(N)$ and $\mathrm{H}_j(k)$, $j\geq 1$, defined by

$$\mathrm{H}_j(n)=\sum_{m=1}^{n}\frac{1}{m^j}. \tag{1}$$

For instance, for $d=3$, one has

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

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

$$\pi_{N,k}=\sum_{N\geq i_1\cdots\geq i_{d-1}>k}\frac{1}{i_1\cdots i_{d-1}}. \tag{3}$$

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

$$\mathrm{A}_{\mathbf{s}}(N)=\sum_{N\geq n_1\geq\cdots\geq n_r>0}\frac{1}{{n_1}^{s_1}\ldots {n_r}^{s_r}}\quad\text{and}\quad \mathrm{H}_{\mathbf{s}}(N)=\sum_{N\geq n_1>\cdots>n_r>0}\frac{1}{{n_1}^{s_1}\ldots {n_r}^{s_r}}. \tag{4}$$

Let us note that there exist explicit relations, given by Hoffman [10] between the $\mathrm{A}_{\mathbf{s}}(N)$ and $\mathrm{H}_{\mathbf{s}}(N)$. 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

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

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

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

$$\begin{aligned} \mathrm{A}_{1,1,1}(N) &= \mathrm{H}_{1,1,1}(N) + \mathrm{H}_{1,2}(N) + \mathrm{H}_{2,1}(N) + \mathrm{H}_3(N), \\ \mathrm{H}_{1,1,1}(N) &= \mathrm{A}_{1,1,1}(N) - \mathrm{A}_{1,2}(N) - \mathrm{A}_{2,1}(N) + \mathrm{A}_3(N). \end{aligned}$$

Therefore, the $\mathrm{A}_{\mathbf{s}}(N)$ are $\mathbb{Z}$-linear combinations on $\mathrm{H}_{\mathbf{s}}(N)$ (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

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

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

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

So, we set the polylogarithmic algebra of $\{\mathrm{P}_{\mathbf{s}}\}_{\mathbf{s}}$, 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 $\{N^k \mathrm{H}_{\mathbf{s}}(N)\}_{\mathbf{s},\, k \in \mathbb{Z}}$ 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 $u = x_0^{s_1 - 1} x_1 \ldots x_0^{s_r - 1} x_1$ over the finite alphabet $X = \{x_0, x_1\}$. In the same way, s can be canonically associated to the word $v = y_{s_1} \ldots y_{s_r}$ over the infinite alphabet $Y = \{y_i\}_{i \geq 1}$. Moreover, in both alphabets, the empty multi-index will correspond to the empty word ϵ. 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

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

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 $v = y_j v'$) is the polynomial recursively defined by

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

$$(\text{resp.} \quad \epsilon \uplus u = u \uplus \epsilon = u \quad \text{and} \quad u \uplus v = y_i(u' \uplus v) + y_j(u \uplus v') + y_{i+j}(u' \uplus v')). \tag{10}$$

Example 2.

$$\begin{aligned} x_0 x_1 \sqcup\!\sqcup x_1 &= x_1 x_0 x_1 + 2 x_0 x_1^2 \\ y_2 \uplus y_1 &= y_1 y_2 + y_2 y_1 + y_3. \end{aligned} \tag{11}$$

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	$\mathcal{Q}_l$	$\mathcal{S}_l$
x_0	x_0	x_0
x_1	x_1	x_1
x_0x_1	$[x_0,\, x_1]$	x_0x_1
${x_0}^2x_1$	$[x_0,\, [x_0,\, x_1]]$	${x_0}^2x_1$
$x_0{x_1}^2$	$[[x_0,\, x_1],\, x_1]$	$x_0{x_1}^2$
${x_0}^3x_1$	$[x_0,\, [x_0,\, [x_0,\, x_1]]]$	${x_0}^3x_1$
$\vdots$	$\vdots$	$\vdots$
${x_0}^3{x_1}^3$	$[x_0,\, [x_0,\, [[[x_0,\, x_1],\, x_1],\, x_1]]]$	${x_0}^3{x_1}^3$
${x_0}^2x_1x_0{x_1}^2$	$[x_0,\, [[x_0,\, x_1],\, [[x_0,\, x_1],\, x_1]]]$	$3{x_0}^3{x_1}^3 + {x_0}^2x_1x_0{x_1}^2$
${x_0}^2{x_1}^2x_0x_1$	$[[x_0,\, [[x_0,\, x_1],\, x_1]],\, [x_0,\, x_1]]$	$6{x_0}^3{x_1}^3 + 3{x_0}^2x_1x_0{x_1}^2 + {x_0}^2{x_1}^2x_0x_1$
${x_0}^2{x_1}^4$	$[x_0,\, [[[[x_0,\, x_1],\, x_1],\, x_1],\, x_1]]$	${x_0}^2{x_1}^4$
$x_0x_1x_0{x_1}^3$	$[[x_0,\, x_1],\, [[[x_0,\, x_1],\, x_1],\, x_1]]$	$4{x_0}^2{x_1}^4 + x_0x_1x_0{x_1}^3$
$x_0{x_1}^5$	$[[[[[x_0,\, x_1],\, x_1],\, x_1],\, x_1],\, x_1]$	$x_0{x_1}^5$

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 ≤ 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*

$$\mathrm{C}_1 = \mathbb{C} \oplus (\mathbb{C}\langle X\rangle \setminus x_0\mathbb{C}\langle X\rangle x_1) \quad \textit{and} \quad \mathrm{C}_2 = \mathbb{C} \oplus (\mathbb{C}\langle Y\rangle \setminus y_1\mathbb{C}\langle Y\rangle)$$

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

$$\begin{aligned}(\mathbb{C}\langle X\rangle, \sqcup\!\sqcup) \simeq \quad & (\mathbb{C}[\mathcal{L}yn(X)], \sqcup\!\sqcup) &= (\mathrm{C}_1[x_0, x_1], \sqcup\!\sqcup),\\ (\mathbb{C}\langle Y\rangle, \uplus) \simeq \quad & (\mathbb{C}[\mathcal{L}yn(Y)], \uplus) &= (\mathrm{C}_2[y_1], \uplus).\end{aligned}$$

Example 4.

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

2.4 Bracket forms and the dual basis

The *bracket form* $\mathcal{Q}_l$ 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

$$\left\{\begin{array}{lcl} \mathcal{Q}_l &=& [\mathcal{Q}_u, \mathcal{Q}_v]\\ \mathcal{Q}_x &=& x \quad \text{for each letter } x \in X,\end{array}\right.$$

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:

$$w = l_1^{\alpha_1} l_2^{\alpha_2} \ldots l_k^{\alpha_k}, \quad l_1 > l_2 > \cdots > l_k, \quad k \geq 0. \tag{12}$$

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]

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

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 $w \in x_0X^*x_1$, one has $\mathcal{S}_w \in x_0\mathbb{Z}\langle X\rangle x_1$.*

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 ω_0 and ω_1 be the two following differential forms

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

One verifies the polylogarithm $\mathrm{Li}_{\mathbf{s}}(z)$, defined by Formula (6), is also the following *iterated integral* with respect to ω_0 and ω_1

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

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

$$\mathrm{Li}_\epsilon(z) = 1, \quad \mathrm{Li}_{x_0}(z) = \log z, \quad \mathrm{Li}_{x_iw}(z) = \int_{0\rightsquigarrow z} \omega_i(t)\,\mathrm{Li}_w(t), \quad \text{for } x_i \in X, w \in X^*. \tag{15}$$

Therefore, Li_w verifies the following identity [4]

$$\forall u, v \in X^*, \qquad \mathrm{Li}_{u \sqcup\!\sqcup v} = \mathrm{Li}_u \mathrm{Li}_v\,. \tag{16}$$

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

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

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

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

satisfying the boundary condition

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

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

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

Example 5 ([5]).

$$\begin{aligned} \mathrm{Li}_{x_0x_1^2}(1-z) &= -\mathrm{Li}_{x_0^2x_1}(z) + \mathrm{Li}_{x_0}(z)\,\mathrm{Li}_{x_0x_1}(z) - \frac{1}{2}\mathrm{Li}_{x_0}^2(z)\,\mathrm{Li}_{x_1}(z) + \zeta(3), \qquad i.e. \\ \mathrm{Li}_{2,1}(1-z) &= -\mathrm{Li}_3(z) + \log(z)\,\mathrm{Li}_2(z) + \frac{1}{2}\log^2(z)\log(1-z) + \zeta(3). \end{aligned}$$

2.6 Harmonic sums

Definition 1. *Let $w = y_{s_1} \ldots y_{s_r} \in Y^*$. For $N \geq r \geq 1$, the harmonic sum $\mathrm{H}_w(N)$ is defined as*

$$\mathrm{H}_w(N) \quad = \quad \sum_{N \geq n_1 > \ldots > n_r > 0} \frac{1}{n_1^{s_1} \ldots n_r^{s_r}}.$$

For $0 \leq N < r$, $\mathrm{H}_w(N) = 0$ and, for the empty word ϵ, we put $\mathrm{H}_\epsilon(N) = 1$, for any $N \geq 0$.

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

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

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

$$\zeta(w) \quad = \quad \sum_{l \geq 1} \frac{\mathrm{H}_{w'}(l-1)}{l^s}, \tag{20}$$

$$\mathrm{H}_w(N+1) - \mathrm{H}_w(N) \quad = \quad (N+1)^{-s} \mathrm{H}_{w'}(N) \tag{21}$$

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

$$\mathrm{H}_{u \,\text{⧢}\, v}(N) \quad = \quad \mathrm{H}_u(N) \mathrm{H}_v(N). \tag{22}$$

3 Generating series

3.1 Definition and first properties

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

$$\mathrm{P}_w(z) = \sum_{N \geq 0} \mathrm{H}_w(N) z^N.$$

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

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 $\{\mathrm{Li}_w\}_{w \in X^*}$ 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 $\mathrm{P}_w(z) = \sum_{N \geq 0} \mathrm{H}_w(N) z^N$ and by using (21),

$$(1-z)\mathrm{P}_w(z) = \mathrm{H}_w(0) + \sum_{N \geq 1} \frac{\mathrm{H}_{w'}(N-1)}{N^s} z^N = \mathrm{Li}_w(z).$$

□

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 $|z| < 1$, $\mathrm{P}_u(z)\mathrm{P}_v(z) = (1-z)^{-1}\mathrm{P}_{u \,\text{ш}\, v}(z)$.*

Example 6. *Since $x_1 \,\text{ш}\, x_0 x_1 = x_1 x_0 x_1 + 2 x_0 x_1^2$ then we get*

$$\mathrm{P}_{1,2}(z) = (1-z)\mathrm{P}_1(z)\mathrm{P}_2(z) - 2\mathrm{P}_{2,1}(z).$$

Proposition 3 allows to extend the definition of P_w over X^* as we have already extended the definition of Li_w over X^*. Moreover,

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

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

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

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

Proof. It follows immediately from Proposition 1. □

Example 7.

$$\mathrm{P}_{2,1}(1-z) = \frac{1-z}{z}\left(-\mathrm{P}_3(z) + \log(z)\mathrm{P}_2(z) - \log^2(z)\mathrm{P}_1(z) + \frac{\zeta(3)}{1-z}\right)$$

Thus,

$$\mathrm{P}_{2,1}(z) = -\frac{z}{1-z}\mathrm{P}_3(1-z) + \frac{z\log(1-z)}{1-z}\mathrm{P}_2(1-z) - \frac{1}{2}\frac{z\log^2(1-z)}{1-z}\mathrm{P}_1(1-z) + \frac{\zeta(3)}{1-z}.$$

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

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

$$\mathrm{P}_w = \sum_{i\in I} \mathrm{P}_{c_i} \odot \mathrm{P}_{y_1}^{\odot i}, \tag{24}$$

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

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

Lemma 2. *Let* $M = \left(m_{i,j}\right)_{1\le i,j\le k}$ *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*

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

Then

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

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

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

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

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

Proposition 5. $\mathrm{H}_{y_1^k}$ *is a combination of* $\{\mathrm{H}_{y_r}\}_{1\leq r<k}$ *which are algebraically independent.*

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

Example 8. *Since*

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

then we have

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

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 $N^a \mathrm{H}_{y_1}^b(N)$). 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 $\mathcal{C}[\{\mathrm{P}_w\}_{w\in Y^*}]$.

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 $1-z$.

$$[z^n](1-z)\mathrm{P}_w(z) \;=\; \mathrm{H}_w(n) - \mathrm{H}_w(n-1). \tag{26}$$

$$[z^n]\frac{\mathrm{P}_w(z)}{1-z} \;=\; \sum_{k=0}^{n} \mathrm{H}_w(k) \tag{27}$$

$$= \begin{cases} (n+1)\mathrm{H}_w(n) - \mathrm{H}_{y_{s-1}w'}(n) \ \text{ if } \ w = y_s w', \text{ with } s \neq 1 \\ (n+1)\mathrm{H}_w(n) - \sum_{j=1}^{n} \mathrm{H}_{w'}(j-1) \ \text{ if } \ w = y_1 w'. \end{cases} \tag{28}$$

and, more generally,

Proposition 6.

$$[z^n](1-z)^k \mathrm{P}_w(z) = \sum_{j=0}^{k} \binom{k}{j} (-1)^j \mathrm{H}_w(n-j) \quad \textit{and} \quad [z^n]\frac{\mathrm{P}_w(z)}{(1-z)^k} = \sum_{n\geq j_1\geq\cdots\geq j_k\geq 0} \mathrm{H}_w(j_k).$$

3.3 Operations on Taylor coefficients of P_w

We are now to find how multiplying or dividing $\mathrm{H}_w(N)$ by N acts on P_w.

3.3.1 A particular case : $w = \epsilon$

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

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

$$n^q = \begin{cases} [z^n](1-z)\mathrm{P}_{-q}(z) & \textit{if} \quad q < 0, \\ [z^n](1-z)^{-1} & \textit{if} \quad q = 0, \\ [z^n]\dfrac{z}{1-z}\mathrm{N}_q\left(\dfrac{1}{1-z}\right) & \textit{if} \quad q > 0, \end{cases}$$

where N_q is defined by the following recurrence

$$\mathrm{N}_0(X) = 1, \quad \textit{and} \quad \mathrm{N}_q(X) = X\left(\sum_{j=0}^{q-1} (-1)^{q-1-j} \binom{q}{j} \mathrm{N}_j(X)\right).$$

Example 9.

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

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 $n^{-k}\mathrm{H}_w(n),\ k$ positive integer, can be identified as follows

$$\begin{aligned} n^{-k}\mathrm{H}_w(n) &= n^{-k}\mathrm{H}_w(n-1) + n^{-s_1-k}\mathrm{H}_{w'}(n-1) && (29)\\ &= [z^n]\,\mathrm{Li}_{y_k w + y_{s_1+k}w'}(z) && (30)\\ &= [z^n][(1-z)\mathrm{P}_{y_k w + y_{s_1+k}w'}(z)]. && (31) \end{aligned}$$

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,

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

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

Definition 4. *For any word $w = x_{i_1}\cdots x_{i_k}$ and for any composition $\mathbf{r} = (r_1,\ldots,r_k)$, 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,*

$$\begin{aligned} &\tau_0(x_0) = x_0\,, && \tau_r(x_1) = x_1,\\ \textit{and, for } r\in\mathbb{N}^*,\quad &\tau_r(x_0) = \theta^r x_0 = 0 \quad \textit{and} && \tau_r(x_1) = \theta^r\frac{zx_1}{1-z} = \frac{r!x_1}{(1-z)^{r+1}}. \end{aligned}$$

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

By applying successively the operator θ to L, we get

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

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

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 $\theta^l\,\mathrm{Li}_w$, for any word $w\in X^*$.

Example 10.

$$\begin{aligned} A_0(z) &= 1,\\ A_1(z) &= x_0 + \frac{z}{1-z}x_1,\\ A_2(z) &= x_0^2 + \frac{z}{1-z}x_0 ⧢ x_1 + \frac{z^2}{(1-z)^2}x_1^2 + \frac{1}{(1-z)^2}x_1. \end{aligned}$$

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

$$\begin{aligned} \theta\,\mathrm{Li}_{x_0^2x_1} &= \left((x_0 + \frac{z}{1-z}x_1)\mathrm{L}(z)\,\Big|\,x_0^2x_1\right)\\ &= \mathrm{Li}_{x_0x_1},\\ \theta^2\,\mathrm{Li}_{x_0^2x_1} &= \left((x_0^2 + \frac{z}{1-z}x_0 ⧢ x_1 + \frac{z^2}{(1-z)^2}x_1^2 + \frac{1}{(1-z)^2}x_1)\mathrm{L}(z)\,\Big|\,x_0^2x_1\right)\\ &= \mathrm{Li}_{x_1}\,. \end{aligned}$$

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

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

Note that the head term of B_l, $l \geq 1$, 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,*

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

Using Leibniz formula, one has

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

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

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

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

$$\begin{aligned}
\theta^2 \mathrm{P}_{x_0^2 x_1}(z) &= \sum_{j=0}^{2} \binom{2}{j} B_j\left(\frac{z}{1-z}\right) \frac{1}{1-z} \theta^{2-j} \operatorname{Li}_w(z) \\
&= \frac{1}{1-z} \operatorname{Li}_{x_1}(z) + 2\frac{z}{1-z}\frac{1}{1-z} \operatorname{Li}_{x_0x_1}(z) + \left(2\left(\frac{z}{1-z}\right)^2 + \frac{z}{1-z}\right) \operatorname{Li}_{x_0^2x_1}(z) \\
&= \mathrm{P}_{x_1}(z) + \frac{2z}{1-z} \mathrm{P}_{x_0x_1}(z) + \frac{z^2+z}{1-z} \mathrm{P}_{x_0^2x_1}(z).
\end{aligned}$$

So, $$n^2 \mathrm{H}_3(n) = [z^n]\left(\mathrm{P}_1(z) + \frac{2z}{1-z}\mathrm{P}_2(z) + \frac{z^2+z}{1-z}\mathrm{P}_3(z)\right).$$

4 The main theorem

Throughout the section, we will write

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

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

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

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

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

to mean

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

For $w = y_1^k$, we know the expression of $[z^N]\mathrm{P}_{y_1^k}(z) = \mathrm{H}_{y_1^k}(N)$ 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

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

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

Example 13. *From Example 8, we can deduce then*

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

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

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

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

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

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

Proof. Considering Corollary 1, we only have firstly to obtain the asymptotic expansion for the case $g(z) = \mathrm{P}_w(z)$. 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 $\{\mathrm{P}_u\}_{u\in X^*}$ 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 $\mathrm{P}_u(z) = \sum_{n\geq 0}\mathrm{H}_u(n)z^n$ and that $\mathrm{P}_{x_0}(z) = (1-z)^{-1}\log(z)$. So, the expected first expansion follows.

From

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

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 $[z^n]\mathrm{P}_{y_1^\beta} = \mathrm{H}_{y_1^\beta}(n)$. For this, we use Lemma 2 which completes our proof. $\square$

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 $(1-z)^k, k\geq 0$ eventually vanish as in the following identity :

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

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 $\sum_{i\in I} b_i n^{\eta_i} \mathrm{H}_1^{\kappa_i}(n)$, we are able to construct the unique function $f \in \mathcal{C}[(\mathrm{P}_w)_{w\in Y^*}]$ such that,*

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

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 $g(z) = \mathrm{P}_w(z)$ directly, it enables to find an asymptotic expansion of $\mathrm{H}_w(N)$, 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 $w \in Y^*$,*

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

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

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

But

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

We find finally, using Example 13 :

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

Otherwise, by Example 6,

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

calculated thanks to Proposition 4. So,

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

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

Example 15. $q_{y_1 y_2} = \zeta(2)\gamma - 2\zeta(3)$ *and* $q_{y_2 y_1} = \zeta(3) = \zeta(2,1)$.

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

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

Example 16. *For* $\mathrm{s} = (1,1,1)$,

$$\begin{aligned}
\mathrm{A}_{1,1,1}(N) &= \mathrm{H}_{1,1,1}(N) + \mathrm{H}_{1,2}(N) + \mathrm{H}_{2,1}(N) + \mathrm{H}_3(N),\\
&= \frac{1}{6}\log^3(N) + \frac{1}{2}\gamma\log^2(N) + \frac{1}{2}[\gamma^2+\zeta(2)]\log(N) - \frac{1}{2}\zeta(2)\gamma + \frac{1}{3}\zeta(3) + \frac{1}{6}\gamma^3 + \frac{1}{4}\frac{\log^2(N)}{N}\\
&+ \frac{1}{2}(\gamma-1)\frac{\log(N)}{N} + \frac{1}{4}[\gamma^2-2\gamma+\zeta(2)]\frac{1}{N} - \frac{1}{24}\frac{\log^2(N)}{N^2} + \frac{1}{24}(9-2\gamma)\frac{\log(N)}{N^2} + \mathrm{O}\left(\frac{1}{N^2}\right).
\end{aligned}$$

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