ALGEBRAIC COMBINATORICS

Hiroaki Nakamura

Demi-shuffle duals of Magnus polynomials in a free associative algebra

Volume 6, issue 4 (2023), p. 929-939.
https://doi.org/10.5802/alco.287

Algebraic Combinatorics is published by The Combinatorics Consortium
and is a member of the Centre Mersenne for Open Scientific Publishing
www.tccpublishing.org www.centre-mersenne.org
e-ISSN: 2589-5486

Algebraic Combinatorics
Volume 6, issue 4 (2023), p. 929–939
https://doi.org/10.5802/alco.287

Demi-shuffle duals of Magnus polynomials in a free associative algebra

Hiroaki Nakamura

Abstract We study two linear bases of the free associative algebra $\mathbb{Z}\langle X, Y\rangle$: one is formed by the Magnus polynomials of type $(\mathrm{ad}_X^{k_1} Y)\cdots(\mathrm{ad}_X^{k_d} Y)X^k$ and the other is its dual basis (formed by what we call the "demi-shuffle" polynomials) with respect to the standard pairing on the monomials of $\mathbb{Z}\langle X, Y\rangle$. As an application, we derive a formula of Le–Murakami, Furusho type that expresses arbitrary coefficients of a group-like series $J \in \mathbb{C}\langle\langle X, Y\rangle\rangle$ in terms of the "regular" coefficients of J.

1. Introduction

Let R be a commutative integral domain of characteristic 0, and let $R\langle X, Y\rangle$ be the free associative algebra generated over R by two (non-commutative) letters X and Y. For $u, v \in R\langle X, Y\rangle$, we shall write $[u, v]$ to denote the Lie bracket $uv - vu$. In [9], W. Magnus introduced the associative subalgebra $S_X \subset R\langle X, Y\rangle$ generated by (what are called) the elements arising by elimination of X:

$$Y^{(0)} := Y, \quad Y^{(k+1)} := [X, Y^{(k)}] \quad (k = 0, 1, 2, \dots), \tag{1}$$

and showed that S_X is freely generated by the $Y^{(k)}$ $(k = 0, 1, 2, \dots)$. Moreover, he derived that every element Z of $R\langle X, Y\rangle$ can be written uniquely in the form

$$Z = \alpha_0 X^m + s_1 X^{m-1} + \cdots + s_m, \tag{2}$$

where $\alpha_0 \in R$, $s_1, \dots, s_m \in S_X$ (see [9, Hilfssatz 2], [10, Lemma 5.6]). This observation is the first step in the construction of the basic Lie elements (an ordered basis of the free Lie algebra), which are obtained via repeated elimination, and whose powered products in decreasing orders give the Poincaré-Birkoff-Witt basis of the enveloping algebra $R\langle X, Y\rangle$ ([10, Theorem 5.8]). Apparently, this theory was historically a starting point toward subsequent developments of finer constructions of free Lie algebra bases due to Lazard, Hall, Lyndon, Viennot and others (see, e.g., [15, Notes 4.5, 5.7]).

In this note, we however stay on the first step of elimination (2) and look at combinatorial properties of a certain basis $\{\mathsf{M}^{(\mathbf{k})}\}_{\mathbf{k}\in\mathbb{N}_0^{(\infty)}}$ of $R\langle X, Y\rangle$ (to be called the Magnus polynomials below) designed as follows:

Manuscript received 19th December 2021, revised 31st July 2022, accepted 16th December 2022.
Keywords. shuffle product, non-commutative polynomial, group-like series.
Acknowledgements. This work was supported by JSPS KAKENHI Grant #JP20H00115.

ISSN: 2589-5486 http://algebraic-combinatorics.org/

Notation 1.1. Let $\mathbb{N}_0$ denote the set of non-negative integers, and let

$$\mathbb{N}_0^{(\infty)} := \bigcup_{d=0}^{\infty}\left(\prod_{k=1}^{d}\mathbb{N}_0\right)\times\mathbb{N}_0$$

be the collection of finite sequences $\mathbf{k}=(k_1,\ldots,k_d;k_\infty)$ of non-negative integers equipped with a special last entry $k_\infty\in\mathbb{N}_0$. Here, we consider $(;k_\infty)$ also as elements of $\mathbb{N}_0^{(\infty)}$ coming from $d=0$. For $\mathbf{k}\in\mathbb{N}_0^{(\infty)}$, define $|\mathbf{k}|:=\sum_{i=1}^{\infty}k_i=k_1+\cdots+k_d+k_\infty$ (resp. $\mathrm{dep}(\mathbf{k}):=d$), and call it the size (resp. depth) of $\mathbf{k}$.

Definition 1.2 (Magnus polynomial). *For $\mathbf{k}=(k_1,\ldots,k_d;k_\infty)\in\mathbb{N}_0^{(\infty)}$, define*

$$\mathsf{M}^{(\mathbf{k})}:=Y^{(k_1)}\cdots Y^{(k_d)}\cdot X^{k_\infty}\in R\langle X,Y\rangle.$$

We also set $\mathsf{M}^{(;0)}=1$, and $\mathsf{M}^{(;k)}=X^k$ for $k=1,2,\ldots$. Note that $\mathsf{M}^{(k;0)}=Y^{(k)}$ for $k\geqslant 0$.

Example 1.3. $\mathsf{M}^{(1,0;2)}=Y^{(1)}Y^{(0)}X^2=(XY-YX)YX^2=XY^2X^2-YXYX^2$.

It is not difficult to see that the Magnus polynomial $\mathsf{M}^{(\mathbf{k})}\in R\langle X,Y\rangle$ is homogeneous of bidegree $(|\mathbf{k}|,\mathrm{dep}(\mathbf{k}))$ in X and Y.

The above mentioned Magnus expression (2) can then be rephrased as

$$Z=\sum_{\mathbf{k}\in\mathbb{N}_0^{(\infty)}}\alpha_{\mathbf{k}}\,\mathsf{M}^{(\mathbf{k})} \tag{3}$$

with uniquely determined coefficients $\alpha_{\mathbf{k}}\in R$ for any given $Z\in R\langle X,Y\rangle$. In other words, the collection $\{\mathsf{M}^{(\mathbf{k})}\mid\mathbf{k}\in\mathbb{N}_0^{(\infty)}\}$ forms an R-linear basis of $R\langle X,Y\rangle$.

Below in §2, we will construct another R-linear basis $\{\mathsf{S}^{(\mathbf{k})}\mid\mathbf{k}\in\mathbb{N}_0^{(\infty)}\}$ (formed by what we call the "demi-shuffle" polynomials) and show that $\{\mathsf{M}^{(\mathbf{k})}\}_{\mathbf{k}}$ and $\{\mathsf{S}^{(\mathbf{k})}\}_{\mathbf{k}}$ are dual to each other under the standard pairing with respect to the monomials of $R\langle X,Y\rangle$ (Theorem 2.4). We then in §3 shortly generalize the duality to the case of free associative algebras of more variables (Theorem 3.2). In §4, we apply the formation of dual basis to derive a formula of Le–Murakami, Furusho type that expresses arbitrary coefficients of a group-like series $J\in R\langle\langle X,Y\rangle\rangle$ in terms of the "regular" coefficients of J (Theorem 4.1).

2. Demi-shuffle duals and array binomial coefficients

Let W be the subset of $R\langle X,Y\rangle$ formed by the monomials in X,Y together with 1, and call any element of W a word. It is clear that W forms a free monoid by the concatenation product that restricts the multiplication of $R\langle X,Y\rangle$. Each element of $R\langle X,Y\rangle$ is an R-linear combination of words in W. For two elements $u,v\in R\langle X,Y\rangle$, define the standard pairing $\langle u,v\rangle\in R$ so as to extend R-linearly the Kronecker symbol $\langle w,w'\rangle:=\delta_w^{w'}\in\{0,1\}$ for words $w,w'\in W$.

Notation 2.1. We use the notation $w_{\mathbf{k}}:=X^{k_1}Y\cdots X^{k_d}YX^{k_\infty}$ and call it the word associated to $\mathbf{k}=(k_1,\ldots,k_d;k_\infty)\in\mathbb{N}_0^{(\infty)}$. The mapping $\mathbf{k}\mapsto w_{\mathbf{k}}$ gives a bijection from $\mathbb{N}_0^{(\infty)}$ onto W. (Note that $w_{(;0)}=1$.) The standard pairing $\langle w_{\mathbf{k}},w_{\mathbf{k}'}\rangle$ is equal to 0 or 1 according to whether $\mathbf{k}\neq\mathbf{k}'$ or $\mathbf{k}=\mathbf{k}'$.

The purpose of this section is to describe the dual of the Magnus basis $\{\mathsf{M}^{(\mathbf{k})}\}_{\mathbf{k}\in\mathbb{N}_0^{(\infty)}}$ with respect to the standard pairing.

Definition 2.2 (Demi-shuffle polynomial). *For $\mathbf{k}=(k_1,\ldots,k_d;k_\infty)\in\mathbb{N}_0^{(\infty)}$, define*

$$\mathsf{S}^{(\mathbf{k})}:=(\cdots((X^{k_1}Y)ш X^{k_2})Y)ш\cdots)ш X^{k_d})Y)ш X^{k_\infty}\in R\langle X,Y\rangle,$$

where $\sqcup\!\sqcup$ *denotes the usual shuffle product. We also set* $\mathsf{S}^{(;0)} = 1$*, and* $\mathsf{S}^{(;k)} = X^k$ *for* $k = 1, 2, \ldots$*. Note that* $\mathsf{S}^{(k;0)} = X^k Y$ *for* $k \geqslant 0$*.*

The construction of $\mathsf{S}^{(\mathbf{k})}$ can be interpreted as forming the linear sum of all words obtained from the word $w_{\mathbf{k}} = X^{k_1}Y \cdots X^{k_d}YX^{k_\infty}$ by consecutively applying "left shuffles" of the X letters and "concatenations" of the Y letters in $w_{\mathbf{k}}$.

Example 2.3. Here are a few examples: $\mathsf{S}^{(0,1;0)} = (Y \sqcup\!\sqcup X)Y = YXY + XYY$; $\mathsf{S}^{(1,1;0)} = ((XY) \sqcup\!\sqcup X)Y = XYXY + 2XXYY$; $\mathsf{S}^{(1,0,1;0)} = (((XY)Y) \sqcup\!\sqcup X)Y = XYYXY + XYXY^2 + 2X^2Y^3$. Using the first identity, one can also compute

$$\begin{aligned}\mathsf{S}^{(0,1;1)} &= ((Y \sqcup\!\sqcup X)Y) \sqcup\!\sqcup X = (YXY + XYY) \sqcup\!\sqcup X\\ &= (YXYX + 2YXXY + XYXY) + (XYYX + XYXY + 2XXYY)\\ &= 2XXYY + 2XYXY + XYYX + 2YXXY + YXYX.\end{aligned}$$

Theorem 2.4 (Duality). *For* $\mathbf{t}, \mathbf{k} \in \mathbb{N}_0^{(\infty)}$*, we have*

$$\langle \mathsf{S}^{(\mathbf{t})}, \mathsf{M}^{(\mathbf{k})} \rangle = \delta_{\mathbf{t}}^{\mathbf{k}}.$$

Here $\delta_{\mathbf{t}}^{\mathbf{k}}$ *is the Kronecker symbol, i.e., designating* 0 *or* 1 *according to whether* $\mathbf{t} \neq \mathbf{k}$ *or* $\mathbf{t} = \mathbf{k}$ *respectively.*

Before going to the proof of the above theorem, we introduce the following notation.

Definition 2.5 (Array binomial coefficient). *For* $\mathbf{t}, \mathbf{k} \in \mathbb{N}_0^{(\infty)}$ *with* $\operatorname{dep}(\mathbf{t}) = \operatorname{dep}(\mathbf{k})$*,* $|\mathbf{t}| = |\mathbf{k}|$*, define*

$$\binom{\mathbf{t}}{\mathbf{k}} := \binom{t_1}{k_1}\binom{t_1 + t_2 - k_1}{k_2} \cdots \binom{t_1 + \cdots t_d - k_1 - \cdots - k_{d-1}}{k_d}, \tag{4}$$

where $\mathbf{t} = (t_1, \ldots, t_d, t_\infty)$*,* $\mathbf{k} = (k_1, \ldots, k_d, k_\infty)$*. We understand* $\binom{\mathbf{t}}{\mathbf{k}} = 1$ *if* $\mathbf{t} = \mathbf{k} = (;N)$ *for some* $N \in \mathbb{N}_0$*. We set* $\binom{\mathbf{t}}{\mathbf{k}} := 0$ *if either* $\operatorname{dep}(\mathbf{t}) \neq \operatorname{dep}(\mathbf{k})$ *or* $|\mathbf{t}| \neq |\mathbf{k}|$ *holds.*

Remark 2.6. The special case $\binom{N,0,\ldots,0;0}{k_1,k_2,\ldots,k_d;k_\infty}$ is the same as the usual multinomial coefficient $\binom{N}{k_1,k_2,\ldots,k_d,k_\infty}$ in combinatorics. Note also that $\binom{\mathbf{t}}{\mathbf{k}} \neq 0$ implies $t_\infty \leqslant k_\infty$, as the last factor of $\binom{\mathbf{t}}{\mathbf{k}}$ could survive only when $(t_1 + \cdots t_d - k_1 - \cdots - k_{d-1}) - k_d = k_\infty - t_\infty \geqslant 0$.

It turns out that the array binomial coefficients give the expansion of $\mathsf{S}^{(\mathbf{t})}$ as a linear sum of the monomials in W. Recall that, for $\mathbf{t} = (t_1, \ldots, t_d, t_\infty) \in \mathbb{N}_0^{(\infty)}$, $w_{\mathbf{t}}$ denotes the word $X^{t_1}YX^{t_2}Y \cdots X^{t_d}YX^{t_\infty} \in W$.

Lemma 2.7 (Monomial expansion).

$$\mathsf{S}^{(\mathbf{k})} = \sum_{\mathbf{t} \in \mathbb{N}_0^{(\infty)}} \binom{\mathbf{t}}{\mathbf{k}} w_{\mathbf{t}}.$$

Proof. Without loss of generality, it suffices to show $\langle w_{\mathbf{t}}, \mathsf{S}^{(\mathbf{k})} \rangle = \binom{\mathbf{t}}{\mathbf{k}}$ in the case $(N :=)\, |\mathbf{t}| = |\mathbf{k}|$ and $(d :=) \operatorname{dep}(\mathbf{t}) = \operatorname{dep}(\mathbf{k})$. The assertion is trivial when $d = 0$, as then $\mathbf{k} = \mathbf{t} = (;N)$, $\mathsf{S}^{(\mathbf{k})} = X^N = w_{\mathbf{t}}$ and $\binom{\mathbf{t}}{\mathbf{k}} = 1$. For $d > 0$, we argue by induction on d. Suppose $d = 1$, $\mathbf{k} = (k_1; k_\infty)$ and $\mathbf{t} = (t_1; t_\infty)$. Then

$$\mathsf{S}^{(\mathbf{k})} = (X^{k_1}Y) \sqcup\!\sqcup X^{k_\infty} = \sum_{i=0}^{k_\infty} (X^{k_1} \sqcup\!\sqcup X^i) Y X^{k_\infty - i} = \sum_{i=0}^{k_\infty} \binom{k_1 + i}{k_1} X^{k_1+i} Y X^{k_\infty - i}.$$

Since $N = k_1 + k_\infty = t_1 + t_\infty$, we have $\langle w_{\mathbf{t}}, \mathsf{S}^{(\mathbf{k})}\rangle = \binom{k_1+k_\infty-t_\infty}{k_1} = \binom{t_1}{k_1}$. Suppose $d > 1$ with $\mathbf{k} = (k_1, \dots, k_d; k_\infty)$ and $\mathbf{t} = (t_1, \dots, t_d; t_\infty)$. Write $\mathbf{k}' = (k_1, \dots, k_{d-1}; 0) \in \mathbb{N}_0^{(\infty)}$. Then

$$\begin{aligned}\mathsf{S}^{(\mathbf{k})} &= (((\mathsf{S}^{(\mathbf{k}')}Y)⧢X^{k_d})Y)⧢X^{k_\infty} \\ &= \sum_{i=0}^{k_\infty} \mathsf{S}^{(\mathbf{k}')}Y(X^{k_d}⧢X^i)YX^{k_\infty-i} \qquad \text{(associativity of ⧢)} \\ &= \sum_{i=0}^{k_\infty}\sum_{\mathbf{t}'}\binom{\mathbf{t}'}{\mathbf{k}'}\binom{k_d+i}{k_d} w_{\mathbf{t}'}X^{k_d+i}YX^{k_\infty-i},\end{aligned}$$

where $\mathbf{t}' = (t_1', \dots, t_{d-1}'; t_d') \in \mathbb{N}_0^{(\infty)}$ runs over those tuples with $t_1' + \dots + t_d' = |\mathbf{k}'|$ so that $\mathsf{S}^{(\mathbf{k}')}$ is expressed as $\sum_{\mathbf{t}'}\binom{\mathbf{t}'}{\mathbf{k}'}w_{\mathbf{t}'}$ by the induction hypothesis on $\mathrm{dep}(\mathbf{k}') = d-1$. The coefficient of $w_{\mathbf{t}}$ in $\mathsf{S}^{(\mathbf{k})}$ can be found in the above summand where $k_\infty - i = t_\infty$, $t_d' + k_d + i = t_d$ and $t_s' = t_s$ $(s = 1, \dots, d-1)$, hence

$$\langle w_{\mathbf{t}}, \mathsf{S}^{(\mathbf{k})}\rangle = \binom{t_1}{k_1}\cdots\binom{t_1+\cdots t_{d-1}-k_1-\cdots-k_{d-2}}{k_{d-1}}\cdot\binom{k_d+k_\infty-t_\infty}{k_d}.$$

Since $N = |\mathbf{k}| = |\mathbf{t}|$, we have $k_d + k_\infty - t_\infty = t_1 + \cdots t_d - k_1 - \cdots - k_{d-1}$. This establishes the formula $\langle w_{\mathbf{t}}, \mathsf{S}^{(\mathbf{k})}\rangle = \binom{\mathbf{t}}{\mathbf{k}}$. □

Remark 2.8. It would be worth noting that Lemma 2.7 can be derived from counting $\langle w_{\mathbf{t}}, \mathsf{S}^{(\mathbf{k})}\rangle$ as the number of certain shufflings of letters in $w_{\mathbf{k}} = X^{k_1}Y\cdots X^{k_d}YX^{k_\infty}$ to produce $w_{\mathbf{t}} = X^{t_1}Y\cdots X^{t_d}YX^{t_\infty}$. Assume $|\mathbf{t}| = |\mathbf{k}|$ and $\mathrm{dep}(\mathbf{t}) = \mathrm{dep}(\mathbf{k})$, and consider letters Y as partitions between groups of letters X in $w_{\mathbf{k}}$ and in $w_{\mathbf{t}}$. Then $\langle w_{\mathbf{t}}, \mathsf{S}^{(\mathbf{k})}\rangle$ is the number of ways of moving some letters X in $w_{\mathbf{k}}$ to the left (beyond any number of Y's) to form the word $w_{\mathbf{t}}$ without changing orders between X's from the same group in $w_{\mathbf{k}}$. We count this number by enumerating branches of possibilities for choosing places of X's in $w_{\mathbf{t}}$ for those moved from $w_{\mathbf{k}}$ group by group. The first binomial factor $\binom{t_1}{k_1}$ of (4) is the number of ways to choose k_1 places for X's (coming from the first group in $w_{\mathbf{k}}$) in the first group $X^{t_1}Y$ of $w_{\mathbf{t}}$. The second binomial factor $\binom{t_1+t_2-k_1}{k_2}$ of (4) represents the number of ways to choose k_2 places for X's (coming from the second group $YX^{k_2}Y$ in $w_{\mathbf{k}}$) in the first two groups $X^{t_1}YX^{t_2}Y$ of $w_{\mathbf{t}}$ where the already occupied k_1 places in the previous step are prohibited from being chosen. We continue the process in the same way. For each given $i \in \{2, \dots, d\}$, suppose that destinations of X's in $X^{t_1}Y\cdots X^{t_{i-1}}$ from $X^{k_1}Y\cdots YX^{k_{i-1}}Y$ have already been chosen. Then, the i-th binomial factor $\binom{t_1+\cdots t_i-k_1-\cdots-k_{i-1}}{k_i}$ of (4) represents the number of ways to choose k_i places for X's (coming from the i-th group $YX^{k_i}Y$ in $w_{\mathbf{k}}$) in $X^{t_1}Y\cdots YX^{t_i}Y$ (the first i groups of $w_{\mathbf{t}}$): there are $t_1 + \cdots + t_i$ places for X in $X^{t_1}Y\cdots YX^{t_i}Y$, but already $k_1 + \cdots + k_{i-1}$ places are occupied by earlier choices. Performing the process until $i = d$ verifies the desired identity $\langle w_{\mathbf{t}}, \mathsf{S}^{(\mathbf{k})}\rangle = \binom{\mathbf{t}}{\mathbf{k}}$.

Proof of Theorem 2.4. From the formula $Y^{(k)} = \sum_{i=0}^{k}(-1)^i\binom{k}{i}X^{k-i}YX^i$ ([9, (4)]), it is not difficult to see that the expansion of the Magnus polynomial in monomials is given by

$$\mathsf{M}^{(\mathbf{k})} = \sum_{\mathbf{t}\in\mathbb{N}_0^{(\infty)}}\begin{Bmatrix}\mathbf{k}\\ \mathbf{t}\end{Bmatrix}w_{\mathbf{t}} \tag{5}$$

with

(6)
$$\begin{Bmatrix}\mathbf{k}\\ \mathbf{t}\end{Bmatrix} := (-1)^{\sum_{i=1}^{d}(d-i+1)(k_i-t_i)}\binom{k_1}{k_1-t_1}\binom{k_2}{k_1+k_2-t_1-t_2}\cdots\binom{k_d}{\sum_{i=1}^{d}(k_i-t_i)}$$

for $\mathbf{t} := (t_1,\dots,t_d;t_\infty)$ and $\mathbf{k} := (k_1,\dots,k_d;k_\infty)$. Since we have $\langle \mathsf{S}^{(\mathbf{t})}, \mathsf{M}^{(\mathbf{k})}\rangle = \sum_{\mathbf{u}\in\mathbb{N}_0^{(\infty)}}\langle \mathsf{S}^{(\mathbf{t})}, w_{\mathbf{u}}\rangle\langle \mathsf{M}^{(\mathbf{k})}, w_{\mathbf{u}}\rangle$, it suffices to show

$$\sum_{\mathbf{u}}\begin{Bmatrix}\mathbf{k}\\ \mathbf{u}\end{Bmatrix}\binom{\mathbf{u}}{\mathbf{t}} = \delta^{\mathbf{t}}_{\mathbf{k}}. \tag{7}$$

Noting that a non-zero pairing $\langle \mathsf{S}^{(\mathbf{t})}, \mathsf{M}^{(\mathbf{k})}\rangle$ occurs only when $|\mathbf{t}|=|\mathbf{k}|$ and $\mathrm{dep}(\mathbf{t}) = \mathrm{dep}(\mathbf{k})$, we may assume without loss of generality that $\mathbf{u}$ in the above summation also runs over those with the fixed size $N := |\mathbf{t}| = |\mathbf{k}|$ and depth $d := \mathrm{dep}(\mathbf{t}) = \mathrm{dep}(\mathbf{k})$. Then, the summation $\sum_{\mathbf{u}}$ with $\mathbf{u} = (u_1,\dots,u_d;u_\infty)$ has d independent parameters $u_1,\dots,u_d$ that determine $u_\infty = N - \sum_{i=1}^{d} u_i$. We may also regard each u_i as running over $\mathbb{Z}$, as the coefficients $\left\{\begin{smallmatrix}\mathbf{k}\\ \mathbf{u}\end{smallmatrix}\right\}$, $\binom{\mathbf{u}}{\mathbf{t}}$ vanish when their combinatorial meaning is lost. Then, in the summation $\sum_{(u_1,\dots,u_d)\in\mathbb{Z}^d}$ in (7), the partial factor of summation involved with the last parameter u_d can be factored out in the form:

$$\begin{aligned}&\sum_{u_d\in\mathbb{Z}}(-1)^{-u_d}\binom{k_d}{u_d+\sum_{i=1}^{d-1}(u_i-k_i)}\binom{u_d+\sum_{i=1}^{d-1}(u_i-t_i)}{t_d}\\ &= (-1)^{\sum_{i=1}^{d-1}(u_i-k_i)-k_d}\binom{\sum_{i=1}^{d-1}(k_i-t_i)}{t_d-k_d}.\end{aligned}$$

(Use [5, (5.24)].) Repeating this process inductively on d, we eventually find

$$\langle \mathsf{S}^{(\mathbf{t})}, \mathsf{M}^{(\mathbf{k})}\rangle = \binom{0}{t_1-k_1}\binom{k_1-t_1}{t_2-k_2}\binom{k_1+k_2-t_1-t_2}{t_3-k_3}\cdots\binom{\sum_{i=1}^{d-1}(k_i-t_i)}{t_d-k_d}$$

which is equal to $\delta^{\mathbf{k}}_{\mathbf{t}}$ as desired. □

Corollary 2.9. *Each element $u \in R\langle X,Y\rangle$ can be written as*

$$u = \sum_{\mathbf{k}\in\mathbb{N}_0^{(\infty)}}\langle \mathsf{S}^{(\mathbf{k})}, u\rangle\, \mathsf{M}^{(\mathbf{k})} = \sum_{\mathbf{k}\in\mathbb{N}_0^{(\infty)}}\langle \mathsf{M}^{(\mathbf{k})}, u\rangle\, \mathsf{S}^{(\mathbf{k})}.$$

Note that only a finite number of summands are nonzero in either summation above.

3. Generalization to the case $R\langle X, Y_1, Y_2, \cdots\rangle$

It is not difficult to generalize the above duality in $R\langle X,Y\rangle$ (Theorem 2.4) to similar duality in $R\langle X, Y_\lambda\rangle_{\lambda\in\Lambda}$ for Λ a nonempty index set, viz. in the associative algebra freely generated by the symbols X, Y_λ ($\lambda\in\Lambda$) over R. In fact, introducing

$$Y_\lambda^{(0)} := Y_\lambda, \quad Y_\lambda^{(k+1)} := [X, Y_\lambda^{(k)}] \quad (\lambda\in\Lambda, k = 0,1,2,\dots), \tag{8}$$

which are called the elements arising by elimination of X, Magnus ([9, Hilfssatz 2], [10, Lemma 5.6]) showed that every element Z of $R\langle X, Y_\lambda\rangle_{\lambda\in\Lambda}$ has the unique expression (2) with S_X the subalgebra freely generated by the $Y_\lambda^{(k)}$ ($k\in\mathbb{N}_0, \lambda\in\Lambda$).

Definition 3.1 (Depth-varied Magnus/demi-shuffle polynomials and monomials). *Let d be a positive integer. For $\mathbf{k} = (k_1,\dots,k_d;k_\infty) \in \mathbb{N}_0^{(\infty)}$ and a finite sequence $\boldsymbol{\lambda} = (\lambda_1,\dots,\lambda_d)\in\Lambda^d$, define*

$$\mathsf{M}^{(\mathbf{k},\boldsymbol{\lambda})} := Y_{\lambda_1}^{(k_1)}\cdots Y_{\lambda_d}^{(k_d)}\cdot X^{k_\infty};$$

$$\mathsf{S}^{(\mathbf{k},\boldsymbol{\lambda})} := (\cdots((X^{k_1}Y_{\lambda_1})\sqcup X^{k_2})Y_{\lambda_2})\sqcup\cdots\sqcup)X^{k_d})Y_{\lambda_d})\sqcup X^{k_\infty};$$
$$w_{\mathbf{k},\boldsymbol{\lambda}} := X^{k_1}Y_{\lambda_1}\cdots X^{k_d}Y_{\lambda_d}X^{k_\infty}.$$

For $d=0$ with $\mathbf{k}=(;k)$, $\boldsymbol{\lambda}=()$, we simply set $w_{(;k),()} = \mathsf{M}^{((;k),())} = \mathsf{S}^{((;k),())} = X^k$.

Note that the monomials $w_{\mathbf{k},\boldsymbol{\lambda}}$ ($\mathbf{k}\in\mathbb{N}_0^{(\infty)}$, $\boldsymbol{\lambda}\in\Lambda^{\mathrm{dep}(\mathbf{k})}$) form an R-linear basis of $R\langle X, Y_\lambda\rangle_{\lambda\in\Lambda}$. Let us write $\langle\ ,\ \rangle$ for the standard pairing defined by the Kronecker symbol with respect to these monomials.

Theorem 3.2 (Duality). *For $\mathbf{t},\mathbf{k}\in\mathbb{N}_0^{(\infty)}$ and $\boldsymbol{\lambda}\in\Lambda^{\mathrm{dep}(\mathbf{t})}$, $\boldsymbol{\mu}\in\Lambda^{\mathrm{dep}(\mathbf{k})}$, we have*

$$\langle \mathsf{S}^{(\mathbf{t},\boldsymbol{\lambda})}, \mathsf{M}^{(\mathbf{k},\boldsymbol{\mu})}\rangle = \delta^{(\mathbf{k},\boldsymbol{\mu})}_{(\mathbf{t},\boldsymbol{\lambda})}.$$

Here $\delta^{(\mathbf{k},\boldsymbol{\mu})}_{(\mathbf{t},\boldsymbol{\lambda})}$ is the Kronecker symbol, i.e., designating 1 or 0 according to whether the pairs $(\mathbf{t},\boldsymbol{\lambda})$ and $(\mathbf{k},\boldsymbol{\mu})$ coincide or not respectively.

Proof. Given a fixed $\boldsymbol{\lambda}=(\lambda_1,\dots,\lambda_d)\in\Lambda^d$, let $V_{\boldsymbol{\lambda}}$ be the R-linear subspace of $R\langle X,Y_\lambda\rangle_{\lambda\in\Lambda}$ generated by the monomials $\{w_{\mathbf{k},\boldsymbol{\lambda}}\mid \mathbf{k}\in\mathbb{N}_0^{(\infty)}, \mathrm{dep}(\mathbf{k})=d\}$. It is obvious that if $\boldsymbol{\lambda}\neq\boldsymbol{\mu}$ then $V_{\boldsymbol{\lambda}}$ and $V_{\boldsymbol{\mu}}$ are mutually orthogonal under the standard pairing $\langle\ ,\ \rangle$. Since $\mathsf{M}^{(\mathbf{k},\boldsymbol{\mu})}\in V_{\boldsymbol{\mu}}$, $\mathsf{S}^{(\mathbf{t},\boldsymbol{\lambda})}\in V_{\boldsymbol{\lambda}}$, we only need to look at the case $\boldsymbol{\mu}=\boldsymbol{\lambda}\in\Lambda^d$. Consider the R-linear subspace V_d of $R\langle X,Y\rangle$ generated by $\{w_{\mathbf{k}}\mid \mathbf{k}\in\mathbb{N}_0^{(\infty)}, \mathrm{dep}(\mathbf{k})=d\}$. Then, the mapping $w_{\mathbf{k}}\mapsto w_{\mathbf{k},\boldsymbol{\lambda}}$ defines an isometry, i.e., an R-linear isomorphism $\phi_{\boldsymbol{\lambda}}: V_d\xrightarrow{\sim} V_{\boldsymbol{\lambda}}$ preserving $\langle\ ,\ \rangle$. The assertion then follows at once from Theorem 2.4 after observing $\phi_{\boldsymbol{\lambda}}(\mathsf{S}^{(\mathbf{t})})=\mathsf{S}^{(\mathbf{t},\boldsymbol{\lambda})}$ and $\phi_{\boldsymbol{\lambda}}(\mathsf{M}^{(\mathbf{k})})=\mathsf{M}^{(\mathbf{k},\boldsymbol{\lambda})}$. □

4. Application to a formula of Le–Murakami and Furusho type

In this section, we assume that R is a field and consider $R\langle X,Y\rangle$ as a subalgebra of the ring of non-commutative formal power series $R\langle\langle X,Y\rangle\rangle$, where a standard comultiplication Δ is defined by setting $\Delta(a)=1\otimes a+a\otimes 1$ for $a\in\{X,Y\}$. An element $J\in R\langle\langle X,Y\rangle\rangle$ is called group-like if it has constant term 1 and satisfies $\Delta(J)=J\otimes J$. There are many group-like elements: for example, the subgroup multiplicatively generated by $\exp(X)$ and $\exp(Y)$ in $R\langle\langle X,Y\rangle\rangle^\times$ consists of group-like elements and forms a free group of rank 2.

Theorem 4.1 (Le–Murakami, Furusho type formula). *Let $J\in R\langle\langle X,Y\rangle\rangle$ be a group-like element in the form*

$$J=\sum_{\mathbf{k}\in\mathbb{N}_0^{(\infty)}} c_{\mathbf{k}} w_{\mathbf{k}},$$

and write c_X for the coefficient $c_{(;1)}$ of X in J. Then,

$$c_{(k_1,\dots,k_d;k_\infty)} = \sum_{\substack{s,t\geqslant 0\\ s+t=k_\infty}} (-1)^s\frac{(c_X)^t}{t!}\sum_{\substack{s_1,\dots,s_d\geqslant 0\\ s=s_1+\cdots+s_d}}\binom{k_1+s_1}{k_1}\cdots\binom{k_d+s_d}{k_d}c_{(k_1+s_1,\dots,k_d+s_d;0)}.$$

We first prove an elementary identity that will be used for the proof of the above formula.

Lemma 4.2. *Let $\boldsymbol{\kappa}=(k_1,\dots,k_d)\in\mathbb{N}_0^d$ and $\mathbf{s}=(s_1,\dots,s_d)\in\mathbb{Z}^d$ satisfy $s=s_1+\cdots+s_d\geqslant 0$ and $k_i+s_i\geqslant 0$ $(i=1,\dots,d)$. Then, we have*

$$\sum_{\boldsymbol{\tau}\in\mathbb{N}_0^d}\langle \mathsf{S}^{(\boldsymbol{\tau};0)}, w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle\cdot\langle \mathsf{M}^{(\boldsymbol{\tau};0)}, w_{(\boldsymbol{\kappa};s)}\rangle = (-1)^s\binom{k_1+s_1}{k_1}\cdots\binom{k_d+s_d}{k_d}.$$

Proof. We shall compute the left-hand side explicitly as the sum over $\boldsymbol{\tau} \in \mathbb{N}_0^d$ satisfying $\sum_{i=1}^d t_i = \sum_{i=1}^d (k_i + s_i)$ with

$$\langle \mathsf{S}^{(\boldsymbol{\tau};0)}, w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle = \binom{(\boldsymbol{\kappa}+\mathbf{s};0)}{(\boldsymbol{\tau};0)} = \binom{k_1+s_1}{t_1} \cdots \binom{\sum_{i=1}^{d-1}(k_i+s_i) - \sum_{i=1}^{d-2} t_i}{t_{d-1}} \binom{t_d}{t_d}$$

by Lemma 2.7 and with

$$\langle \mathsf{M}^{(\boldsymbol{\tau};0)}, w_{(\boldsymbol{\kappa};s)}\rangle = \left\{ {(\boldsymbol{\tau};0) \atop (\boldsymbol{\kappa};s)} \right\} = (-1)^{s+\sum_{i=1}^{d-1}(d-i)(t_i-k_i)} \binom{t_1}{t_1-k_1} \cdots \binom{t_{d-1}}{\sum_{i=1}^{d-1}(t_i-k_i)} \binom{t_d}{s}$$

by (5) and $s = \sum_{i=1}^d (t_i - k_i)$. Note that, since $\binom{(\boldsymbol{\kappa}+\mathbf{s};0)}{(\boldsymbol{\tau};0)}\left\{ {(\boldsymbol{\tau};0) \atop (\boldsymbol{\kappa};s)} \right\} \neq 0$ only when all entries of $\boldsymbol{\tau} = (t_1, \dots, t_d)$ are nonnegative and $t_1 + \cdots + t_d = \sum_{i=1}^d (k_i + s_i)$ (a constant), the above sum can be taken over the tuples $(t_1, \dots, t_{d-1}) \in \mathbb{Z}^{d-1}$ with entries running as independent integers. Then, the partial summation involved with the last variable t_{d-1} may be factored out as

$$\begin{aligned}
&\sum_{t_{d-1}} (-1)^{t_{d-1}} \binom{\sum_{i=1}^{d-1}(k_i+s_i) - \sum_{i=1}^{d-2} t_i}{t_{d-1}} \binom{t_{d-1}}{\sum_{i=1}^{d-1}(t_i-k_i)} \binom{t_d}{s} \\
&= \sum_{t_{d-1}} (-1)^{t_{d-1}} \binom{\sum_{i=1}^{d-1}(k_i+s_i) - \sum_{i=1}^{d-2} t_i}{\sum_{i=1}^{d-1} k_i - \sum_{i=1}^{d-2} t_i} \binom{\sum_{i=1}^{d-1} s_i}{\sum_{i=1}^{d-1}(t_i-k_i)} \binom{\sum_{i=1}^{d}(k_i+s_i) - \sum_{i=1}^{d-1} t_i}{\sum_{i=1}^{d} s_i} \\
&= \binom{\sum_{i=1}^{d-1}(k_i+s_i) - \sum_{i=1}^{d-2} t_i}{\sum_{i=1}^{d-1} s_i} (-1)^{\sum_{i=1}^{d-1} k_i - \sum_{i=1}^{d-2} t_i} \binom{k_d+s_d}{s_d},
\end{aligned}$$

where [5, (5.21)] is applied for the first equality and [5, (5.24)] for the second. After factoring out the constant $\binom{k_d+s_d}{s_d}$ and repeating the similar process with the other variables $t_{d-2}, \dots, t_1$ consecutively, we eventually obtain the asserted formula. Below in Note 4.3, we also provide an alternative proof of the lemma free from intricate use of [5, (5.21),(5.24)]. ☐

Proof of Theorem 4.1. We argue in the beautiful framework exploited in Reutenauer's book [15, 1.5] using the complete tensor product

$$\mathscr{A} = R\langle\langle X, Y\rangle\rangle \bar{\otimes} R\langle\langle X, Y\rangle\rangle$$

equipped with a product induced from the shuffle product (resp. the concatenation product) on the left (resp. right) of $\bar{\otimes}$. Recall that the ring of R-linear endomorphisms $\mathrm{End}_R R\langle\langle X, Y\rangle\rangle$ can be embedded into $\mathscr{A}$ by $f \mapsto \sum_{w \in W} w \otimes f(w)$, and that the product of $\mathscr{A}$ restricts to the convolution product of $\mathrm{End}_R R\langle\langle X, Y\rangle\rangle$ defined by $f * g := \mathrm{conc} \circ (f \otimes g) \circ \Delta$ (where "conc" means concatenation of left and right sides of $\otimes$). Note that, for $f \in \mathrm{End}_R R\langle\langle X, Y\rangle\rangle$ and $J \in R\langle\langle X, Y\rangle\rangle$, we have $f(J) = \sum_{w \in W} \langle w, J\rangle f(w)$.

Since, by Corollary 2.9, every word w can be written as $\sum_{\mathbf{t} \in \mathbb{N}_0^{(\infty)}} \langle \mathsf{S}^{(\mathbf{t})}, w\rangle \mathsf{M}^{(\mathbf{t})}$, the element of $\mathscr{A}$ corresponding to the identity id $\in \mathrm{End}_R R\langle\langle X, Y\rangle\rangle$ is:

$$\begin{aligned}
\sum_{w \in W} w \otimes w &= \sum_{w} w \otimes \sum_{\mathbf{t}} \langle \mathsf{S}^{(\mathbf{t})}, w\rangle \mathsf{M}^{(\mathbf{t})} = \sum_{\mathbf{t}} (\sum_{w} \langle \mathsf{S}^{(\mathbf{t})}, w\rangle w) \otimes \mathsf{M}^{(\mathbf{t})} \\
&= \sum_{\mathbf{t}} \mathsf{S}^{(\mathbf{t})} \otimes \mathsf{M}^{(\mathbf{t})} \\
&= \left(\sum_{d=0}^{\infty} \sum_{\boldsymbol{\tau} \in \mathbb{N}_0^d} \mathsf{S}^{(\boldsymbol{\tau};0)} \otimes \mathsf{M}^{(\boldsymbol{\tau};0)} \right) \cdot \left(\sum_{t=0}^{\infty} X^t \otimes X^t \right),
\end{aligned}$$

where we have used $\mathsf{S}^{(\mathbf{t})}=\mathsf{S}^{(\boldsymbol{\tau};t)}=\mathsf{S}^{(\boldsymbol{\tau};0)}ш X^t$ and $\mathsf{M}^{(\mathbf{t})}=\mathsf{M}^{(\boldsymbol{\tau};t)}=\mathsf{M}^{(\boldsymbol{\tau};0)}\cdot X^t$. Observing that both factors of the last expression above correspond to specific R-linear endomorphisms, we can apply id to J as the convolution product of them and find from $\Delta(J)=J\otimes J$ that

$$J=\mathrm{id}(J)=\left(\sum_{d=0}^{\infty}\sum_{\boldsymbol{\tau}\in\mathbb{N}_0^d}\langle\mathsf{S}^{(\boldsymbol{\tau};0)},J\rangle\mathsf{M}^{(\boldsymbol{\tau};0)}\right)\left(\sum_{t=0}^{\infty}\frac{(c_X)^t}{t!}X^t\right). \tag{9}$$

Note here that the pairing of J with $X^t=X^{ш t}/t!$ is equal to $(c_X)^t/t!$, as easily seen from the fact that the specialization $J(X,0)\in R\langle\langle X\rangle\rangle$ at $Y=0$ is a group like element $\exp(c_X\cdot X)$. To complete the proof of Theorem 4.1, given a fixed $\mathbf{k}=(\boldsymbol{\kappa};k_\infty)=(k_1,\dots,k_d;k_\infty)\in\mathbb{N}_0^{(\infty)}$ and $0\leqslant s\leqslant k_\infty$, we compute the coefficient of $w_{(\kappa;s)}=X^{k_1}Y\cdots X^{k_d}YX^s$ in the expansion of the first factor of the above right-hand side as follows:

$$\begin{aligned}\sum_{d=0}^{\infty}\sum_{\boldsymbol{\tau}\in\mathbb{N}_0^d}\langle\mathsf{S}^{(\boldsymbol{\tau};0)},J\rangle\langle\mathsf{M}^{(\boldsymbol{\tau};0)},w_{(\boldsymbol{\kappa};s)}\rangle&=\left\langle\sum_{d=0}^{\infty}\sum_{\boldsymbol{\tau}\in\mathbb{N}_0^d}\langle\mathsf{S}^{(\boldsymbol{\tau};0)},J\rangle\mathsf{M}^{(\boldsymbol{\tau};0)},w_{(\boldsymbol{\kappa};s)}\right\rangle\\ =\left\langle\sum_{d=0}^{\infty}\sum_{\boldsymbol{\tau}\in\mathbb{N}_0^d}\left\langle\mathsf{S}^{(\boldsymbol{\tau};0)},\sum_{\mathbf{u}\in\mathbb{N}_0^{(\infty)}}(J,w_{\mathbf{u}})w_{\mathbf{u}}\right\rangle\mathsf{M}^{(\boldsymbol{\tau};0)},w_{(\boldsymbol{\kappa};s)}\right\rangle&\\ =\sum_{\mathbf{u}}\langle J,w_{\mathbf{u}}\rangle\sum_{d=0}^{\infty}\sum_{\boldsymbol{\tau}\in\mathbb{N}_0^d}\langle\mathsf{S}^{(\boldsymbol{\tau};0)},w_{\mathbf{u}}\rangle\langle\mathsf{M}^{(\boldsymbol{\tau};0)},w_{(\boldsymbol{\kappa};s)}\rangle.&\end{aligned}$$

But since $\langle\mathsf{S}^{(\boldsymbol{\tau};0)},w_{\mathbf{u}}\rangle\langle\mathsf{M}^{(\boldsymbol{\tau};0)},w_{(\boldsymbol{\kappa};s)}\rangle$ survives only when $\mathrm{dep}(\boldsymbol{\tau};0)=\mathrm{dep}(\boldsymbol{\kappa};s)=\mathrm{dep}(\mathbf{u})$ and $|(\boldsymbol{\tau};0)|=|(\boldsymbol{\kappa};s)|=|\mathbf{u}|$, the summation $\sum_{\mathbf{u}}$ in the last expression above occurs only for those $\mathbf{u}$ of the form $(\boldsymbol{\kappa}+\mathbf{s};0)\in\mathbb{N}_0^{(\infty)}$ with $\mathbf{s}=(s_1,\dots,s_d)\in\mathbb{Z}^d$, $s=s_1+\cdots+s_d\geqslant 0$ (cf. also Remark 2.6). Then, it follows from Lemma 4.2 that the last expression above is equal to

$$\sum_{d=0}^{\infty}\sum_{\substack{\mathbf{s}\in\mathbb{N}_0^d\\|(\mathbf{s};0)|=s}}\langle J,w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle(-1)^s\binom{k_1+s_1}{k_1}\cdots\binom{k_d+s_d}{k_d}.$$

(Note: the prescribed condition $\mathbf{s}\in\mathbb{Z}^d$ has been replaced with $\mathbf{s}\in\mathbb{N}_0^d$ because of the a posteriori survivals of binomial factors.) From this and (9) together with $\langle J,w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle=c_{(k_1+s_1,\dots,k_d+s_d;0)}$, we conclude the assertion. □

Note 4.3 (*Alternative proof of Lemma* 4.2). In the right-hand side of Lemma 4.2, the quantity $\binom{k_1+s_1}{k_1}\cdots\binom{k_d+s_d}{k_d}$ appearing there can also be interpreted as the pairing $\langle w_{(k_1,\dots,k_d;0)}ш X^s,w_{(k_1+s_1,\dots,k_d+s_d;0)}\rangle$. Therefore, the assertion of this lemma is equivalent to the identity

$$\sum_{\boldsymbol{\tau}\in\mathbb{N}_0^d}\langle\mathsf{S}^{(\boldsymbol{\tau};0)},w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle\cdot\langle\mathsf{M}^{(\boldsymbol{\tau};0)},w_{(\boldsymbol{\kappa};0)}\cdot X^s\rangle=(-1)^s\langle w_{(\boldsymbol{\kappa};0)}ш X^s,w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle \tag{10}$$

for $\boldsymbol{\kappa}=(k_1,\dots,k_d)\in\mathbb{N}_0^d$, $\mathbf{s}=(s_1,\dots,s_d)\in\mathbb{Z}^d$ satisfying $s=s_1+\cdots+s_d\geqslant 0$ and $\boldsymbol{\kappa}+\mathbf{s}\in\mathbb{N}_0^d$. We now give an alternative proof for it using the Magnus/demi-shuffle duality. First, by Corollary 2.9, we have $w_{(\boldsymbol{\kappa};0)}=\sum_{\mathbf{r}}\langle\mathsf{M}^{(\mathbf{r})},w_{(\boldsymbol{\kappa};0)}\rangle\mathsf{S}^{(\mathbf{r})}$ and $w_{(\boldsymbol{\kappa}+\mathbf{s};0)}=\sum_{\mathbf{t}}\langle\mathsf{S}^{(\mathbf{t})},w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle\mathsf{M}^{(\mathbf{t})}$ so that the right-hand side of (10) can be written as

$$(-1)^s\langle w_{(\boldsymbol{\kappa};0)}ш X^s,w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle \tag{11}$$

$$= (-1)^s \sum_{\mathbf{r},\mathbf{t}\in\mathbb{N}_0^{(\infty)}} \langle \mathsf{S}^{(\mathbf{r})} ⧢ X^s, \mathsf{M}^{(\mathbf{t})}\rangle \langle \mathsf{M}^{(\mathbf{r})}, w_{(\boldsymbol{\kappa};0)}\rangle \langle \mathsf{S}^{(\mathbf{t})}, w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle$$
$$= (-1)^s \sum_{\boldsymbol{\rho}\in\mathbb{N}_0^d} \langle \mathsf{M}^{(\boldsymbol{\rho};0)}, w_{(\boldsymbol{\kappa};0)}\rangle \langle \mathsf{S}^{(\boldsymbol{\rho};s)}, w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle.$$

Here in the second equality, we use the fact that $\langle \mathsf{M}^{(\mathbf{r})}, w_{(\boldsymbol{\kappa};0)}\rangle$ survives only if $\mathbf{r} = (\boldsymbol{\rho}; 0) \in \mathbb{N}_0^{(\infty)}$ for some $\boldsymbol{\rho} \in \mathbb{N}_0^d$ and then apply the duality (Theorem 2.4) to $\langle \mathsf{S}^{(\mathbf{r})} ⧢ X^s, \mathsf{M}^{(\mathbf{t})}\rangle$ with $\mathsf{S}^{(\boldsymbol{\rho};0)} ⧢ X^s = \mathsf{S}^{(\boldsymbol{\rho};s)}$ (cf. Definitions 1.2 and 2.2).

On the other hand, in the left-hand side of (10), one observes that nontrivial terms of the summation arise only from those $\boldsymbol{\tau} = (\tau_1, \dots, \tau_d) \in \mathbb{N}_0^d$ with $\sum_{i=1}^d \tau_i = s + \sum_{i=1}^d \kappa_i$ (a constant). But the last binomial factor in (6) for $\langle \mathsf{M}^{(\boldsymbol{\tau};0)}, w_{(\boldsymbol{\kappa};0)} \cdot X^s\rangle = \left\{\begin{smallmatrix}(\tau_1,\dots,\tau_d;0)\\(\kappa_1,\dots,\kappa_d;s)\end{smallmatrix}\right\}$ equals $\binom{\tau_d}{s}$, which is non-zero only if $\tau_d \geqslant s$. Therefore, the summation $\sum_{\boldsymbol{\tau}}$ may be replaced by $\sum_{\boldsymbol{\rho}}$ with $\boldsymbol{\rho} = \boldsymbol{\tau} - (\mathbf{0}, s)$ in $\mathbb{N}_0^d$ (where $\mathbf{0} \in \mathbb{N}_0^{d-1}$ is the zero vector). Thus, the left-hand side of (10) can be written as

$$\sum_{\boldsymbol{\tau}\in\mathbb{N}_0^d} \langle \mathsf{S}^{(\boldsymbol{\tau};0)}, w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle \cdot \langle \mathsf{M}^{(\boldsymbol{\tau};0)}, w_{(\boldsymbol{\kappa};0)} \cdot X^s\rangle \tag{12}$$
$$= \sum_{\boldsymbol{\rho}\in\mathbb{N}_0^d} \langle \mathsf{S}^{(\boldsymbol{\rho}+(\mathbf{0},s);0)}, w_{(\boldsymbol{\kappa}+\mathbf{s};0)}\rangle \cdot \langle \mathsf{M}^{(\boldsymbol{\rho}+(\mathbf{0},s);0)}, w_{(\boldsymbol{\kappa};s)}\rangle.$$

Comparing summands of the above (11) and (12) for individual $\boldsymbol{\rho} \in \mathbb{N}_0^d$ in view of coefficients of monomial expansions of demi-shuffle/Magnus polynomials (Lemma 2.7 and (5)), we reduce the formula (10) to the following elementary identity for $\boldsymbol{\kappa} = (k_i)$, $\boldsymbol{\rho} = (r_i) \in \mathbb{N}_0^d$ and $\mathbf{s} = (s_i) \in \mathbb{Z}^d$ satisfying $\sum_{i=1}^d k_i = \sum_{i=1}^d r_i$, $\mathbf{s} + \boldsymbol{\kappa} \in \mathbb{N}_0^d$ and $s := \sum_{i=1}^d s_i \geqslant 0$:

$$\binom{(\boldsymbol{\kappa}+\mathbf{s};0)}{(\boldsymbol{\rho};s)} \left\{\begin{matrix}(\boldsymbol{\rho};0)\\(\boldsymbol{\kappa};0)\end{matrix}\right\} = (-1)^s \binom{(\boldsymbol{\kappa}+\mathbf{s};0)}{(\boldsymbol{\rho}+(\mathbf{0},s);0)} \left\{\begin{matrix}(\boldsymbol{\rho}+(\mathbf{0},s);0)\\(\boldsymbol{\kappa},s)\end{matrix}\right\}. \tag{13}$$

This is an immediate consequence of definitions of these symbols $\left\{\begin{smallmatrix}*\\*\end{smallmatrix}\right\}$, $\binom{*}{*}$. (Observe that only difference between the corresponding symbols occurs from the last binomial coefficient in (4) and (6).) □

Example 4.4. The following shows an output of a group-like element $J = \sum_{w\in W} c_w w$ of $R\langle\langle X, Y\rangle\rangle$ with the shuffle relation (which is necessary and sufficient for group-likeness due to Ree [14]). It was computed using the software [11], and shows terms up to total degree 4.

$$J = 1 + c_X X + c_Y Y + \frac{c_X^2 XX}{2} + c_{XY} XY + (c_X c_Y - c_{XY})\, YX + \frac{c_Y^2\, YY}{2} + \frac{c_X^3 XXX}{6}$$
$$+ c_{XXY} XXY + (c_X c_{XY} - 2c_{XXY})\, XYX + c_{XYY} XYY + \left(\frac{1}{2}c_X^2 c_Y - c_X c_{XY} + c_{XXY}\right) YXX$$
$$+ (c_{XY} c_Y - 2c_{XYY})\, YXY + \left(\frac{1}{2}c_X c_Y^2 - c_{XY} c_Y + c_{XYY}\right) YYX + \frac{c_Y^3\, YYY}{6}$$
$$+ \frac{c_X^4 XXXX}{24} + c_{XXXY} XXXY + (c_X c_{XXY} - 3c_{XXXY})\, XXYX + c_{XXYY} XXYY$$
$$+ \left(\frac{1}{2}c_X^2 c_{XY} - 2c_X c_{XXY} + 3c_{XXXY}\right) XYXX + \left(\frac{c_{XY}^2}{2} - 2c_{XXYY}\right) XYXY$$
$$+ \left(c_X c_{XYY} - \frac{c_{XY}^2}{2}\right) XYYX + c_{XYYY} XYYY + \left(\frac{1}{6}c_X^3 c_Y - \frac{1}{2}c_X^2 c_{XY} + c_X c_{XXY} - c_{XXXY}\right) YXXX$$
$$+ \left(c_{XXY} c_Y - \frac{c_{XY}^2}{2}\right) YXXY + \left(c_X c_{XY} c_Y - 2c_X c_{XYY} - 2c_{XXY} c_Y + \frac{1}{2}c_{XY}^2 + 2c_{XXYY}\right) YXYX$$

$$+ (c_{XYY}c_Y - 3c_{XYYY})\, YXYY + \left(\frac{1}{4}c_X^2c_Y^2 - c_Xc_{XY}c_Y + c_Xc_{XYY} + c_{XXY}c_Y - c_{XXYY}\right) YYXX$$
$$+ \left(\frac{1}{2}c_{XY}c_Y^2 - 2c_{XYY}c_Y + 3c_{XYYY}\right) YYXY + \left(\frac{1}{6}c_Xc_Y^3 - \frac{1}{2}c_{XY}c_Y^2 + c_{XYY}c_Y - c_{XYYY}\right) YYYX$$
$$+ \frac{c_Y^4\, YYYY}{24} \quad + \quad \text{(terms of degree} \geqslant 5).$$

In the above computation, one observes that the coefficient c_{XYXY} is expressed by lower, simpler coefficients of J. This does not follow from Theorem 4.1; however, it does reflect the fact that $XYXY$ is not a Lyndon word. Discussions on the most economical expression using only the coefficients of Lyndon words can be found in [12].

Note 4.5. In the modern theory of multiple zeta values, a certain standard solution $G_0^z(X,Y) \in \mathbb{C}\langle\langle X,Y\rangle\rangle$ to the KZ-equation on $z \in \mathbb{C} - \{0,1\}$ is known as the generating function for the multiple polylogarithms (MPL). It is also used to define the Drinfeld associator $\Phi(X,Y) \in \mathbb{C}\langle\langle X,Y\rangle\rangle$. The coefficients of $w_{(k_1,\dots,k_d;0)}$ in $\Phi(X,Y)$ (resp. in $G_0^z(X,Y)$) are regular multiple zeta values (resp. regular MPL) of multi-index $(k_1,\dots,k_d)$, but the other coefficients are in general not. Le–Murakami [7] and Furusho [4] derived formulas that express all coefficients of $\Phi(X,Y)$ and $G_0^z(X,Y)$ by those "regular" coefficients explicitly. In [13, Remark 2], the author posed a question if something similar could be the case for the "ℓ-adic Galois associator $f_\sigma^z(X,Y) \in \mathbb{Q}_\ell\langle\langle X,Y\rangle\rangle$", in which context the analytic theory of KZ-equation is unavailable as of yet. Since $f_\sigma^z(X,Y)$ is by definition a group-like element, the above Theorem 4.1 answers the question affirmatively.

Note 4.6. A noteworthy notion closely related to our $\mathsf{S}^{(\mathbf{k})}$, $\mathsf{S}^{(\mathbf{k},\boldsymbol{\lambda})}$ is the free Zinbiel (or, dual Leibniz) algebra studied by J.-L. Loday [8], I. Dokas [2], F. Chapoton [1] and others. Let V be a vector space with a basis $\mathfrak{B} = \{X_0, X_1, \dots\}$ and $T(V)$ be the tensor algebra (free associative algebra) generated by the letters in $\mathfrak{B}$. Loday introduced the "half-shuffle" product $\prec$ in $T(V)$ as the linear extension of the binary product on words given by:

$$(x_0x_1\cdots x_p) \prec (x_{p+1}\cdots x_{p+q}) := x_0 \cdot \big((x_1\cdots x_p) ⧢ (x_{p+1}\cdots x_{p+q})\big),$$

where x_i are letters in $\mathfrak{B}$ ($i = 0,\dots,p+q$). It is worth noting that, while the usual shuffle product $w ⧢ w' = w \prec w' + w' \prec w$ is associative (and commutative), the half-shuffle product $\prec$ is not even associative; however, it does satisfy $(w_1 \prec w_2) \prec w_3 = w_1 \prec (w_2 \prec w_3) + w_1 \prec (w_3 \prec w_2)$. We may relate the "Zinbiel monomials" with our demi-shuffle polynomials $\mathsf{S}^{(\mathbf{k},\boldsymbol{\lambda})}$ in Definition 3.1 as follows. Write $* \mapsto \overline{*}$ for the anti-automorphism of $R\langle X, Y_\lambda\rangle_{\lambda\in\Lambda}$ reversing the order of letters in each word, e.g., $\overline{XXY_\lambda} = Y_\lambda XX$. Then,

$$\overline{\mathsf{S}^{(\mathbf{k},\boldsymbol{\lambda})}} = X^{k_\infty} ⧢ \big(\dots\big(Y_{\lambda_d}X^{k_d} \prec \big(Y_{\lambda_{d-1}}X^{k_{d-1}} \prec \big(\cdots \prec \big(Y_{\lambda_2}X^{k_2} \prec Y_{\lambda_1}X^{k_1}\big)\big)\dots\big) \tag{14}$$

for $\mathbf{k} = (k_1,\dots,k_d;k_\infty) \in \mathbb{N}_0^{(\infty)}$, $\boldsymbol{\lambda} = (\lambda_1,\dots,\lambda_d) \in \Lambda^d$. These polynomials also appeared in [6, Proposition 5.10] to illustrate the coefficients (of the main factor) of a solution of the KZ-equation expanded in $(\mathrm{ad}_{-X}^{k_1}Y)\cdots(\mathrm{ad}_{-X}^{k_d}Y)$. We also learned from a paper by L. Foissy and F. Patras [3] that already in M.-P. Schützenberger's work [16] there is an axiomatic treatment of half-shuffle combinatorics on words called the "algèbre de shuffle".

Calling $\mathsf{S}^{(\mathbf{k})}$, $\mathsf{S}^{(\mathbf{k},\boldsymbol{\lambda})}$ "demi-shuffles" as in Definitions 2.2, 3.1, and reserving "semi-shuffle" for the name of anything else, might keep a moderate distance from the already overloaded term "half-shuffle" of the operation $\prec$ in the literature.

Acknowledgements. The author is grateful to Hidekazu Furusho, whose hinting at a positive answer to the question posed in [13, Remark 2] led toward the form of Theorem 4.1 of the present paper, and for valuable comments and information on what is mentioned in part of Note 4.6. He also thanks Densuke Shiraishi for stimulating discussions which made him aware of various open problems around ℓ-adic Galois multiple polylogarithms. The author would like to express his gratitude to the referees for useful comments that helped to improve the presentation of this paper.

References

[1] Frédéric Chapoton, *Zinbiel algebras and multiple zeta values*, Doc. Math. **27** (2022), 519–533.

[2] Ioannis Dokas, *Zinbiel algebras and commutative algebras with divided powers*, Glasg. Math. J. **52** (2010), no. 2, 303–313.

[3] Loïc Foissy and Frédéric Patras, *Natural endomorphisms of shuffle algebras*, Internat. J. Algebra Comput. **23** (2013), no. 4, 989–1009.

[4] Hidekazu Furusho, *p-adic multiple zeta values. I. p-adic multiple polylogarithms and the p-adic KZ equation*, Invent. Math. **155** (2004), no. 2, 253–286.

[5] Ronald L. Graham, Donald E. Knuth, and Oren Patashnik, *Concrete mathematics*, second ed., Addison-Wesley Publishing Company, Reading, MA, 1994, A foundation for computer science.

[6] Vincel Hoang Ngoc Minh, *On the solutions of the universal differential equation with three regular singularities (on solutions of KZ_3)*, Confluentes Math. **11** (2019), no. 2, 25–64.

[7] Thang Tu Quoc Le and Jun Murakami, *Kontsevich's integral for the Kauffman polynomial*, Nagoya Math. J. **142** (1996), 39–65.

[8] Jean-Louis Loday, *Cup-product for Leibniz cohomology and dual Leibniz algebras*, Math. Scand. **77** (1995), no. 2, 189–196.

[9] Wilhelm Magnus, *Über Beziehungen zwischen höheren Kommutatoren*, J. Reine Angew. Math. **177** (1937), 105–115.

[10] Wilhelm Magnus, Abraham Karrass, and Donald Solitar, *Combinatorial group theory*, second ed., Dover Publications, Inc., Mineola, NY, 2004, Presentations of groups in terms of generators and relations.

[11] Maplesoft, a division of Waterloo Maple Inc.., *Maple (2021 version)*, Waterloo, Ontario, `https://hadoop.apache.org`.

[12] Hoang Ngoc Minh, Michel Petitot, and Joris Van Der Hoeven, *Shuffle algebra and polylogarithms*, Discrete Math. **225** (2000), no. 1-3, 217–230, Formal power series and algebraic combinatorics (Toronto, ON, 1998).

[13] Hiroaki Nakamura, *Some aspects of arithmetic functions in Grothendieck-Teichmüller theory*, Oberwolfach Rep. **18** (2021), no. 1, 700–702, part of "Homotopic and geometric Galois theory. Abstracts from the workshop held March 7–13, 2021 (online meeting)".

[14] Rimhak Ree, *Lie elements and an algebra associated with shuffles*, Ann. of Math. (2) **68** (1958), 210–220.

[15] Christophe Reutenauer, *Free Lie algebras*, London Mathematical Society Monographs. New Series, vol. 7, The Clarendon Press, Oxford University Press, New York, 1993, Oxford Science Publications.

[16] Marcel-Paul Schützenberger, *Sur une propriété combinatoire des demi-groupes libres*, C. R. Acad. Sci. Paris **245** (1957), 16–18.

Hiroaki Nakamura, Osaka University, Department of Mathematics, Graduate School of Science, Toyonaka, Osaka 560-0043 (Japan)
E-mail : `nakamura@math.sci.osaka-u.ac.jp`
Url : `http://www4.math.sci.osaka-u.ac.jp/~nakamura`