

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

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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 $(\text{ad}_X^{k_1} Y) \cdots (\text{ad}_X^{k_d} Y) X^k$ 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 show 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 .

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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 [8], 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 :

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

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

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

where $\alpha_0 \in R$, $s_1, \dots, s_m \in S_X$ (see [8, Hilfssatz 2], [9, Lemma 5.6]). This observation is the first step preceding to repeated elimination for the construction of the basic Lie elements (an ordered basis of free Lie algebra) whose powered products in decreasing orders give Poincaré-Birkoff-Witt basis of the enveloping algebra $R\langle X, Y \rangle$ ([9, 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 (cf. e.g., [15, Notes 4.5, 5.7]).

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

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 $\mathbf{k} = (k_1, \dots, k_d; k_\infty)$ 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 $|\mathbf{k}| := \sum_{i=1}^{\infty} k_i = k_1 + \dots + k_d + k_\infty$ (resp. $\text{dep}(\mathbf{k}) := d$), and call it the size (resp. depth) of \mathbf{k} .

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

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

We also set $\mathbf{M}^{(;0)} = 1$, $\mathbf{M}^{(;k)} = X^k$ ($k = 1, 2, \dots$). Note that $\mathbf{M}^{(k;0)} = Y^{(k)}$ for $k \geq 0$.

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

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

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

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

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

Below in §2, we will construct another R -linear basis $\{\mathbf{S}^{(\mathbf{k})} \mid \mathbf{k} \in \mathbb{N}_0^{(\infty)}\}$ (formed by what we call the ‘demi-shuffle’ polynomials) and show that $\{\mathbf{M}^{(\mathbf{k})}\}_{\mathbf{k}}$ and $\{\mathbf{S}^{(\mathbf{k})}\}_{\mathbf{k}}$ 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 $w_{\mathbf{k}} := X^{k_1}Y \dots X^{k_d}YX^{k_\infty}$ and call it the word associated to $\mathbf{k} = (k_1, \dots, k_d; k_\infty) \in \mathbb{N}_0^{(\infty)}$. The mapping $\mathbf{k} \mapsto w_{\mathbf{k}}$ gives a bijection between $\mathbb{N}_0^{(\infty)}$ 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 $\{M^{(\mathbf{k})}\}_{\mathbf{k} \in \mathbb{N}_0^{(\infty)}}$ with respect to the standard pairing.

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

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

where \sqcup denotes the usual shuffle product. We also set $S^{(:,0)} = 1$, $S^{(:,k)} = X^k$ ($k = 1, 2, \dots$). Note that $S^{(k;0)} = X^k Y$ for $k \geq 0$.

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

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

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

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

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

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 $\text{dep}(\mathbf{t}) = \text{dep}(\mathbf{k})$, $|\mathbf{t}| = |\mathbf{k}|$, define

$$(4) \quad \binom{\mathbf{t}}{\mathbf{k}} := \binom{t_1}{k_1} \binom{t_1 + t_2 - k_1}{k_2} \dots \binom{t_1 + \dots + t_d - k_1 - \dots - k_{d-1}}{k_d},$$

where $\mathbf{t} = (t_1, \dots, t_d, t_\infty)$, $\mathbf{k} = (k_1, \dots, k_d, k_\infty)$. 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 $\text{dep}(\mathbf{t}) \neq \text{dep}(\mathbf{k})$ or $|\mathbf{t}| \neq |\mathbf{k}|$ holds.

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

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

Lemma 2.7 (Monomial expansion).

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

Proof. Without loss of generality, it suffices to show $\langle w_{\mathbf{t}}, \mathbf{S}(\mathbf{k}) \rangle = \binom{\mathbf{t}}{\mathbf{k}}$ in the case $(N :=) |\mathbf{t}| = |\mathbf{k}|$ and $(d :=) \text{dep}(\mathbf{t}) = \text{dep}(\mathbf{k})$. The assertion is trivial when $d = 0$, as then $\mathbf{k} = \mathbf{t} = (; N)$, $\mathbf{S}(\mathbf{k}) = X^N = w_{\mathbf{t}}$ 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

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

Since $N = k_1 + k_\infty = t_1 + t_\infty$, we have $\langle w_{\mathbf{t}}, \mathbf{S}(\mathbf{k}) \rangle = \binom{k_1+k_\infty-t_\infty}{k_1} = \binom{t_1}{k_1}$. 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

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

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 $\mathbf{S}(\mathbf{k}')$ is expressed as $\sum_{\mathbf{t}'} \binom{\mathbf{t}'}{\mathbf{k}'}$ by the induction hypothesis on $\text{dep}(\mathbf{k}') = d-1$. The coefficient of $w_{\mathbf{t}}$ in $\mathbf{S}(\mathbf{k})$ 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

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

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

Remark 2.8. It would be worth noting that Lemma 2.7 can be derived from counting $\langle w_{\mathbf{t}}, \mathbf{S}(\mathbf{k}) \rangle$ as the number of certain shuffling of letters in $w_{\mathbf{k}} = X^{k_1}Y \dots X^{k_d}Y X^{k_\infty}$ to produce $w_{\mathbf{t}} = X^{t_1}Y \dots X^{t_d}Y X^{t_\infty}$. Assume $|\mathbf{t}| = |\mathbf{k}|$ and $\text{dep}(\mathbf{t}) = \text{dep}(\mathbf{k})$, and consider letters Y as partitions between groups of letters X 's in $w_{\mathbf{k}}$ and in $w_{\mathbf{t}}$. Then $\langle w_{\mathbf{t}}, \mathbf{S}(\mathbf{k}) \rangle$ 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 already occupied k_1 places in the previous step are prohibited to choose. We continue the process in the same way. For each given $i \in \{2, \dots, d\}$, suppose that destinations of X 's in $X^{t_1}Y \dots X^{t_{i-1}}$ from $X^{k_1}Y \dots YX^{k_{i-1}}Y$ has already been chosen. Then, the i -th binomial factor $\binom{t_1+\dots+t_i-k_1-\dots-k_{i-1}}{k_i}$ 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 $X^{t_1}Y \dots YX^{t_i}Y$ (the first i groups of $w_{\mathbf{t}}$): There are $t_1 + \dots + t_i$ places for X in $X^{t_1}Y \dots YX^{t_i}Y$ but already $k_1 + \dots + k_{i-1}$ places are occupied by earlier choices. Performing the process till $i = d$ verifies the desired identity $\langle w_{\mathbf{t}}, \mathbf{S}(\mathbf{k}) \rangle = \binom{\mathbf{t}}{\mathbf{k}}$.

Proof of Theorem 2.4. It is not difficult to see from the formula $Y^{(k)} = \sum_{i=0}^k (-1)^i \binom{k}{i} X^{k-i} Y X^i$ ([8, (4)]) that the expansion of the Magnus polynomial in monomials is given by

$$(5) \quad M^{(\mathbf{k})} = \sum_{\mathbf{t} \in \mathbb{N}_0^{(\infty)}} \left\{ \begin{matrix} \mathbf{k} \\ \mathbf{t} \end{matrix} \right\} w_{\mathbf{t}}$$

with

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

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

$$(7) \quad \sum_{\mathbf{u}} \left\{ \begin{matrix} \mathbf{k} \\ \mathbf{u} \end{matrix} \right\} \binom{\mathbf{u}}{\mathbf{t}} = \delta_{\mathbf{k}}^{\mathbf{t}}.$$

Noting that non-zero pairing $\langle S^{(\mathbf{t})}, M^{(\mathbf{k})} \rangle$ occurs only when $|\mathbf{t}| = |\mathbf{k}|$, $\text{dep}(\mathbf{t}) = \text{dep}(\mathbf{k})$, without loss of generality, we may assume that \mathbf{u} in the above summation also runs over those with the fixed size $N := |\mathbf{t}| = |\mathbf{k}|$ and depth $d := \text{dep}(\mathbf{t}) = \text{dep}(\mathbf{k})$. 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 running over \mathbb{Z} , as the coefficients $\left\{ \begin{matrix} \mathbf{k} \\ \mathbf{u} \end{matrix} \right\}$, $\binom{\mathbf{u}}{\mathbf{t}}$ vanish when 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

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

which is equal to $\delta_{\mathbf{k}}^{\mathbf{t}}$ as desired. \square

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

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

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

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

It is not difficult to generalize the above duality in $R\langle X, Y \rangle$ (Theorem 2.4) to similar duality in $R\langle X, Y_\lambda \rangle_{\lambda \in \Lambda}$ (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

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

that are called the elements arising by elimination of X , Magnus ([8, Hilfssatz 2], [9, 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

$$\begin{aligned} M^{(\mathbf{k}, \boldsymbol{\lambda})} &:= Y_{\lambda_1}^{(k_1)} \dots Y_{\lambda_d}^{(k_d)} \cdot X^{k_\infty}; \\ S^{(\mathbf{k}, \boldsymbol{\lambda})} &:= (\dots ((X^{k_1} Y_{\lambda_1}) \sqcup X^{k_2}) Y_{\lambda_2}) \sqcup \dots \sqcup X^{k_d}) Y_{\lambda_d}) \sqcup X^{k_\infty}; \\ w_{\mathbf{k}, \boldsymbol{\lambda}} &:= X^{k_1} Y_{\lambda_1} \dots X^{k_d} Y_{\lambda_d} X^{k_\infty}. \end{aligned}$$

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

Note that the monomials $w_{\mathbf{k}, \boldsymbol{\lambda}}$ ($\mathbf{k} \in \mathbb{N}_0^{(\infty)}$, $\boldsymbol{\lambda} \in \Lambda^{\text{dep}(\mathbf{k})}$) form an R -linear basis of $R\langle X, Y_\lambda \rangle_{\lambda \in \Lambda}$. Let us write $\langle \cdot, \cdot \rangle$ 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 $\boldsymbol{\lambda} \in \Lambda^{\text{dep}(\mathbf{t})}$, $\boldsymbol{\mu} \in \Lambda^{\text{dep}(\mathbf{k})}$, we have

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

Here $\delta_{(\mathbf{t}, \boldsymbol{\lambda})}^{(\mathbf{k}, \boldsymbol{\mu})}$ 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_λ be the R -linear subspace of $R\langle X, Y_\lambda \rangle_{\lambda \in \Lambda}$ generated by the monomials $\{w_{\mathbf{k}, \boldsymbol{\lambda}} \mid \mathbf{k} \in \mathbb{N}_0^{(\infty)}, \text{dep}(\mathbf{k}) = d\}$. It is obvious that if $\boldsymbol{\lambda} \neq \boldsymbol{\mu}$ then V_λ and V_μ are mutually orthogonal under the standard pairing $\langle \cdot, \cdot \rangle$. Since $M^{(\mathbf{k}, \boldsymbol{\mu})} \in V_\mu$, $S^{(\mathbf{t}, \boldsymbol{\lambda})} \in V_\lambda$, 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 $\{w_{\mathbf{k}} \mid \mathbf{k} \in \mathbb{N}_0^{(\infty)}, \text{dep}(\mathbf{k}) = d\}$. Then, the mapping $w_{\mathbf{k}} \mapsto w_{\mathbf{k}, \boldsymbol{\lambda}}$ defines an isometry, i.e., an R -linear isomorphism $\phi_\lambda : V_d \xrightarrow{\sim} V_\lambda$ preserving $\langle \cdot, \cdot \rangle$. The assertion then follows at once from Theorem 2.4 after observing $\phi_\lambda(S^{(\mathbf{t})}) = S^{(\mathbf{t}, \boldsymbol{\lambda})}$ and $\phi_\lambda(M^{(\mathbf{k})}) = M^{(\mathbf{k}, \boldsymbol{\lambda})}$. \square

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,

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

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 $s = s_1 + \dots + s_d \geq 0$ and $k_i + s_i \geq 0$ ($i = 1, \dots, d$). Then, we have*

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

Proof. We shall compute the LHS 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

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

by Lemma 2.7 and with

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

by (5) and $s = \sum_{i=1}^d (t_i - k_i)$. Note that, since $\binom{(\boldsymbol{\kappa} + \mathbf{s}; 0)}{(\boldsymbol{\tau}; 0)} \left\{ \binom{(\boldsymbol{\tau}; 0)}{(\boldsymbol{\kappa}; s)} \right\} \neq 0$ only when all entries of $\boldsymbol{\tau} = (t_1, \dots, t_d)$ are nonnegative and $t_1 + \dots + t_d = \sum_{i=1}^d (k_i + s_i)$ (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)]. \square

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

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

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 endomorphism $\text{End}_R R\langle\langle X, Y \rangle\rangle$ can be embedded into \mathcal{A} by $f \mapsto \sum_{w \in W} w \otimes f(w)$, and that the product of \mathcal{A} restricts to the convolution product of $\text{End}_R R\langle\langle X, Y \rangle\rangle$ defined by $f * g := \text{conc} \circ (f \otimes g) \circ \Delta$ ('conc' means concatenation of left and right sides of \otimes). Note that, for $f \in \text{End}_R R\langle\langle X, Y \rangle\rangle$ 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 $\sum_{\mathbf{t} \in \mathbb{N}_0^{(\infty)}} \langle \mathbf{S}^{(\mathbf{t})}, w \rangle \mathbf{M}^{(\mathbf{t})}$, the element of \mathcal{A} corresponding to the identity $\text{id} \in \text{End}_R R\langle\langle X, Y \rangle\rangle$ is:

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

where used are $\mathbf{S}^{(\mathbf{t})} = \mathbf{S}^{(\boldsymbol{\tau};t)} = \mathbf{S}^{(\boldsymbol{\tau};0)} \sqcup X^t$ and $\mathbf{M}^{(\mathbf{t})} = \mathbf{M}^{(\boldsymbol{\tau};t)} = \mathbf{M}^{(\boldsymbol{\tau};0)} \cdot X^t$. Observing that both factors of the above last side 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

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

Note here that the pairing of J with $X^t = X^{\sqcup t}/t!$ 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 settle 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 $0 \leq s \leq k_{\infty}$, we compute the coefficient of $w_{(\boldsymbol{\kappa};s)} = X^{k_1} Y \cdots X^{k_d} Y X^s$ in the expansion of the first factor of the above right hand side as follows:

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

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

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

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

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 $s = s_1 + \cdots + s_d \geq 0$ 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 $w_{(\boldsymbol{\kappa}; 0)} = \sum_{\mathbf{r}} \langle \mathbf{M}^{(\mathbf{r})}, w_{(\boldsymbol{\kappa}; 0)} \rangle \mathbf{S}^{(\mathbf{r})}$ and $w_{(\boldsymbol{\kappa}+\mathbf{s}; 0)} = \sum_{\mathbf{t}} \langle \mathbf{S}^{(\mathbf{t})}, w_{(\boldsymbol{\kappa}+\mathbf{s}; 0)} \rangle \mathbf{M}^{(\mathbf{t})}$ so that the RHS of (10) can be written as

$$(11) \quad \begin{aligned} & (-1)^s \langle w_{(\boldsymbol{\kappa}; 0)} \sqcup X^s, w_{(\boldsymbol{\kappa}+\mathbf{s}; 0)} \rangle \\ &= (-1)^s \sum_{\mathbf{r}, \mathbf{t} \in \mathbb{N}_0^{(\infty)}} \langle \mathbf{S}^{(\mathbf{r})} \sqcup X^s, \mathbf{M}^{(\mathbf{t})} \rangle \langle \mathbf{M}^{(\mathbf{r})}, w_{(\boldsymbol{\kappa}; 0)} \rangle \langle \mathbf{S}^{(\mathbf{t})}, w_{(\boldsymbol{\kappa}+\mathbf{s}; 0)} \rangle \\ &= (-1)^s \sum_{\boldsymbol{\rho} \in \mathbb{N}_0^d} \langle \mathbf{M}^{(\boldsymbol{\rho}; 0)}, w_{(\boldsymbol{\kappa}; 0)} \rangle \langle \mathbf{S}^{(\boldsymbol{\rho}; s)}, w_{(\boldsymbol{\kappa}+\mathbf{s}; 0)} \rangle. \end{aligned}$$

Here in the second equality, we use the fact that $\langle \mathbf{M}^{(\mathbf{r})}, w_{(\boldsymbol{\kappa}; 0)} \rangle$ 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 $\langle \mathbf{S}^{(\mathbf{r})} \sqcup X^s, \mathbf{M}^{(\mathbf{t})} \rangle$ with $\mathbf{S}^{(\boldsymbol{\rho}; 0)} \sqcup X^s = \mathbf{S}^{(\boldsymbol{\rho}; s)}$ (cf. Definitions 1.2 and 2.2).

On the other hand, in the LHS of (10), one observes that nontrivial terms of the summation arise only from those $\boldsymbol{\tau} = (\tau_1, \dots, \tau_d) \in \mathbb{N}_0^d$ subject to $\sum_{i=1}^d \tau_i = s + \sum_{i=1}^d \kappa_i$ (constant). But then, the last binomial factor in (6) for $\langle \mathbf{M}^{(\boldsymbol{\tau}; 0)}, w_{(\boldsymbol{\kappa}; 0)} \cdot X^s \rangle = \left\{ \binom{\tau_1, \dots, \tau_d; 0}{\kappa_1, \dots, \kappa_d; s} \right\}$ equals $\binom{\tau_d}{s}$ which is non-zero only if $\tau_d \geq s$. 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 $\mathbf{0} \in \mathbb{N}_0^{d-1}$: the zero vector). Thus, the LHS of (10) can be written as

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

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 $s := \sum_{i=1}^d s_i \geq 0$:

$$(13) \quad \binom{(\boldsymbol{\kappa} + \mathbf{s}; 0)}{(\boldsymbol{\rho}; s)} \left\{ \binom{(\boldsymbol{\rho}; 0)}{(\boldsymbol{\kappa}; 0)} \right\} = (-1)^s \binom{(\boldsymbol{\kappa} + \mathbf{s}; 0)}{(\boldsymbol{\rho} + (\mathbf{0}, s); 0)} \left\{ \binom{(\boldsymbol{\rho} + (\mathbf{0}, s); 0)}{(\boldsymbol{\kappa}, s)} \right\}$$

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

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]) counted from a computation using software [10] up to total degree 4.

$$\begin{aligned}
J = & 1 + c_X X + c_Y Y + \frac{c_X^2 XX}{2} + c_{XY} XY + (c_X c_Y - c_{XY}) YX + \frac{c_Y^2 YY}{2} + \frac{c_X^3 XXX}{6} \\
& + c_{XXY} XXY + (c_X c_{XY} - 2c_{XXY}) XYX + c_{XYY} XYY + \left(\frac{1}{2} c_X^2 c_Y - c_X c_{XY} + c_{XXY} \right) YXX \\
& + (c_{XY} c_Y - 2c_{XYY}) YXY + \left(\frac{1}{2} c_X c_Y^2 - c_{XY} c_Y + c_{XYY} \right) YYX + \frac{c_Y^3 YYY}{6} \\
& + \frac{c_X^4 XXXX}{24} + c_{XXXY} XXXY + (c_X c_{XXY} - 3c_{XXXY}) XXYX + c_{XXYY} XYYX \\
& + \left(\frac{1}{2} c_X^2 c_{XY} - 2c_X c_{XXY} + 3c_{XXXY} \right) XYXX + \left(\frac{c_{XY}^2}{2} - 2c_{XXYY} \right) XYYX \\
& + \left(c_X c_{XYY} - \frac{c_{XY}^2}{2} \right) XYYX + c_{XYYY} XYYY + \left(\frac{1}{6} c_X^3 c_Y - \frac{1}{2} c_X^2 c_{XY} + c_X c_{XXY} - c_{XXXY} \right) YXXX \\
& + \left(c_{XXY} c_Y - \frac{c_{XY}^2}{2} \right) YXXY + \left(c_X c_{XY} c_Y - 2c_X c_{XYY} - 2c_{XXY} c_Y + \frac{1}{2} c_{XY}^2 + 2c_{XXYY} \right) YXYX \\
& + (c_{XYY} c_Y - 3c_{XYYY}) YXYX + \left(\frac{1}{4} c_X^2 c_Y^2 - c_X c_{XY} c_Y + c_X c_{XYY} + c_{XXY} c_Y - c_{XXYY} \right) YYXX \\
& + \left(\frac{1}{2} c_{XY} c_Y^2 - 2c_{XYY} c_Y + 3c_{XYYY} \right) YYXY + \left(\frac{1}{6} c_X c_Y^3 - \frac{1}{2} c_{XY} c_Y^2 + c_{XYY} c_Y - c_{XYYY} \right) YYYX \\
& + \frac{c_Y^4 YYYY}{24} + (\text{terms of degree } \geq 5).
\end{aligned}$$

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, 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 [6], 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 it could be a similar case for ‘ ℓ -adic Galois associator $f_\sigma^z(X, Y) \in \mathbb{Q}_\ell\langle\langle X, Y \rangle\rangle$ ’, in which context analytic theory of KZ-equation is unavailable 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 $\mathbf{S}^{(\mathbf{k})}$, $\mathbf{S}^{(\mathbf{k}, \lambda)}$ is the free Zinbiel (or, dual Leibniz) algebra studied by J.-L. Loday [7], I. Dookas [2], F. Chapoton [1] et.al. 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:

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

where x_i are letters in \mathfrak{B} ($i = 0, \dots, p+q$). It is remarkable that, while the usual shuffle product $w \sqcup w' = w \prec w' + w' \prec w$ is associative (and commutative), the half-shuffle product \prec is not even associative — however satisfying $(w_1 \prec w_2) \prec w_3 = w_1 \prec (w_2 \prec w_3) + w_1 \prec (w_3 \prec w_2)$. We may relate the ‘Zinbiel monomials’ with our demi-shuffle polynomials $\mathbf{S}^{(\mathbf{k}, \lambda)}$ in Definition 3.1 as follows: Write $* \mapsto \bar{*}$ 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,

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

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 [11, Proposition 5.10] to illustrate the coefficients (of the main factor) of a solution of the KZ-equation expanded in $(\text{ad}_{-X}^{k_1} Y) \cdots (\text{ad}_{-X}^{k_d} Y)$. We also learn from a paper by L. Foissy and F. Patras [3] that already in M.-P. Schützenberger’s work [16] is found an axiomatic treatment of half-shuffle combinatorics on words named “algèbre de shuffle”.

Calling $S(\mathbf{k})$, $S(\mathbf{k}, \boldsymbol{\lambda})$ ‘demi-shuffle’ in Definitions 2.2, 3.1 or reserving ‘semi-shuffle’ for names of anything else might keep a moderate distance from the already overwhelming naming ‘half-shuffle’ of the operation \prec in literature.

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