BINARY SHUFFLE BASES FOR QUASI-SYMMETRIC FUNCTIONS

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Abstract. We construct bases of quasi-symmetric functions whose product rule is given by the shuffle of binary words, as for multiple zeta values in their integral representations, and then extend the construction to the algebra of free quasi-symmetric functions colored by positive integers. As a consequence, we show that the fractions introduced in [Guo and Xie, Ramanujan Jour. 25 (2011) 307-317] provide a realization of this algebra by rational moulds extending that of free quasi-symmetric functions given in [Chapoton et al., Int. Math. Res. Not. IMRN 2008, no. 9, Art. ID rnn018].

1. Introduction

The algebra of Quasi-symmetric functions $QSym(X)$ [7] is the linear span of the expressions

$$M_I(X) := \sum_{n_1<n_2<\ldots<n_r} x_{n_1}^{i_1} x_{n_2}^{i_2} \cdots x_{n_r}^{i_r}, \tag{1}$$

called quasi-monomial functions. Here, $X = \{x_i\}$ is a totally ordered set of mutually commuting variables and $I = (i_1, \ldots, i_r)$ is a finite sequence of positive integers (a composition of degree $n = i_1 + \cdots + i_r$ of M_I).

The M_I are partially symmetric functions (actually, the invariants of a special action of the symmetric group [9]), and the point is that $QSym(X)$ is actually an algebra. The product rule involves an operation on compositions often called quasi-shuffle [11], or stuffle [2], or augmented shuffle [9]. Let $\uplus$ be defined as follows [22]:

$$au \uplus bv = a(u \uplus bv) + b(au \uplus v) + (a \dotplus b)(u \uplus v) \tag{2}$$

$$a \uplus \epsilon = \epsilon \uplus a = a\,, \tag{3}$$

where $a, b \in \mathbb{N}^*$, ϵ is the empty word, $a \dotplus b$ denotes the sum of integers, and u, v are two compositions regarded as words on the alphabet $\mathbb{N}^*$.
Then, given two compositions I and J, we have:

$$M_I M_J = \sum_K \langle K \mid I \uplus J\rangle M_K \tag{4}$$

where the notation $\langle x|y\rangle$ means "the coefficient of x in y". For example:

$$\begin{aligned} M_{21}M_{12} &= 2M_{2112} + M_{2121} + M_{213} + M_{222} \\ &\quad + M_{1212} + 2M_{1221} + M_{123} + M_{141} + M_{312} + M_{321} + M_{33}\,. \end{aligned} \tag{5}$$

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As is well known, this quasi-shuffle, which contains all the terms of the ordinary shuffle $I \sqcup\!\sqcup J$ together with contractions obtained by adding two consecutive parts coming from different terms, defines a structure actually isomorphic to an ordinary shuffle algebra. The best way to see this is to recall that *QSym* is a Hopf algebra, and that its dual is the algebra **Sym** of noncommutative symmetric functions [14, 6]. Since **Sym** can be freely generated by a sequence containing one primitive element P_n in each degree, the dual Q_I of the multiplicative basis $P^I = P_{i_1} \cdots P_{i_r}$ satisfies

$$Q_I Q_J = \sum_K \langle K \mid I \sqcup\!\sqcup J \rangle Q_K \,. \tag{6}$$

Thus, the quasi-shuffle algebra over the positive integers is isomorphic to the shuffle algebra over the same set, and it is straightforward to see that this is true in general [11].

This isomorphism plays an important role in the theory of multiple zeta values (MZV), also called polyzetas or Euler-Zagier sums [23]. Indeed, these are specializations of the quasi-monomial functions obtained by setting

$$x_n = \frac{1}{n} \quad \text{or} \quad x_{-n} = \frac{1}{n} \quad \text{(there are two conventions).} \tag{7}$$

The second convention being more frequent, we shall set

$$\zeta(I) = \sum_{n_1 > n_2 > \ldots > n_r} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_r^{i_r}} \tag{8}$$

so that the convergent ones are those with $i_1 > 1$.

Hence, the convergent MZV satisfy the product rule (4). However, one of the big mysteries of the theory relies on the fact that they also satisfy another product formula, the shuffle relation, which is *not* the shuffle of compositions as in (6). This formula comes from the following integral representation. Let

$$\omega_0(t) = \frac{dt}{t} \quad \text{and} \quad \omega_1(t) = \frac{dt}{1-t} \,. \tag{9}$$

Then, for a composition I of n,

$$\zeta(I) = \int_{0 < t_1 < t_2 \ldots < t_n} \omega_{\epsilon_1}(t_n) \wedge \omega_{\epsilon_2}(t_{n-1}) \wedge \cdots \wedge \omega_{\epsilon_n}(t_1) \tag{10}$$

where ϵ is the word $\epsilon_I = 0^{i_1-1}10^{i_2-1}1 \cdots 0^{i_r-1}1$. Then, a standard property of iterated integrals (often referred to as Chen's lemma) implies that

$$\zeta(I)\zeta(J) = \sum_K \langle \epsilon_K | \epsilon_I \sqcup\!\sqcup \epsilon_J \rangle \zeta(K) \,. \tag{11}$$

The existence of such a formula for a specialization of quasi-symmetric functions raises the question of the existence of a similar one for the generic case. That is, does there exist a basis Z_I of *QSym* such that

$$Z_I Z_J = \sum_K \langle \epsilon_K | \epsilon_I \sqcup\!\sqcup \epsilon_J \rangle Z_K \,? \tag{12}$$

We shall answer this question in three different ways. First, a counting argument shows easily that such bases do exist. This does not however provide a pratical way to construct them. Next, we propose a recusive algorithm allowing to construct such a basis from any basis Q_I satisfying (6). Finally, we describe another construction and we obtain an explicit combinatorial formula for matrices expressing the dual basis X_I of Z_I over the dual basis P_I of any basis Q_I as above.

The interesting point of this last construction is that it involves in a crucial way the Hopf algebra of set partitions **WSym** (symmetric functions in noncommuting variables), and its relations with the commutative combinatorial Hopf algebras exhibited in [10]. Indeed, our matrices are obtained from two simple statistics of set partitions, which are in some way compatible with the Hopf structure. The row sums, for example, yield a known form of the noncommutative Bell polynomials, and the column sums correspond to new analogs of these.

Finally, we extend our construction to $\mathbf{FQSym}^{(\mathbb{N}^*)}$, the algebra of colored free quasi-symmetric functions, with the set of positive integers as color set [15]. Namely, we exhibit bases whose product rule coincides with that of the MZV fractions introduced by Guo and Xin [8], thus providing a realization of this algebra by rational moulds extending that of **FQSym** given in [3].

2. Lyndon words and Lyndon compositions

We shall work in the shuffle algebra $\mathbb{K}_{\sqcup\!\sqcup}\langle a,b\rangle$ over two letters a and b (rather than 0,1), with $a < b$, $\mathbb{K}$ being a field of characteristic 0. We then replace the notation ϵ_I by W_I, so that *e.g.*, $W_{213} = abbaab$.

By Radford's theorem [17], $\mathbb{K}_{\sqcup\!\sqcup}\langle a,b\rangle$ is a polynomial algebra freely generated by Lyndon words. Apart from a, all Lyndon words over a, b end by a b. Words ending by b are in bijection with compositions, and Lyndon words ending by b correspond to Lyndon compositions. Precisely, I is anti-Lyndon (a Lyndon composition for the opposite order on the integers) iff W_I (or ϵ_I) is a Lyndon word.

For example, the Lyndon words of length 6 are

$$aaaaab,\ aaaabb,\ aaabab,\ aaabbb,\ aababb,\ aabbab,\ aabbbb,\ ababbb\ abbbbb, \tag{13}$$

and their encodings by compositions are

$$6,\ 51,\ 42,\ 411,\ 321,\ 312,\ 3111,\ 2211,\ 21111. \tag{14}$$

Since *QSym* is the shuffle algebra over the positive integers, it is a polynomial algebra over (anti-) Lyndon compositions. Hence it is isomorphic to the subalgebra $K_{\sqcup\!\sqcup}\langle a,b\rangle b$ (spanned by words ending by b) of the shuffle algebra over two letters. We then have

Proposition 2.1. *There exists a basis Z_I of QSym satisfying Eq.* (12)*:*

$$Z_I Z_J = \sum_K \langle \epsilon_K | \epsilon_I \sqcup\!\sqcup\, \epsilon_J \rangle Z_K\,.$$

This argument does not yet give a systematic procedure to build a basis with the required properties. An algorithm will be described in the forthcoming section.

3. An algorithmic construction

Our problem is clearly equivalent to the following one: build a basis Y_I of $K_{\sqcup\!\sqcup}\langle a,b\rangle b$ such that

$$Y_I \sqcup\!\sqcup Y_J = \sum_K \langle K \mid I \sqcup\!\sqcup J\rangle Y_K\,. \tag{15}$$

For an anti-Lyndon composition L, we set $Y_L = W_L$ (a Lyndon word). Thus, we start with

$$Y_1 = b, \quad Y_2 = ab, \quad Y_3 = aab, \quad Y_{21} = abb, \quad Y_{211} = abbb, \ldots \tag{16}$$

and applying iteratively (15), we obtain

$$Y_1 \sqcup\!\sqcup Y_1 = 2Y_{11} = b \sqcup\!\sqcup b = 2bb, \tag{17}$$

$$Y_1 \sqcup\!\sqcup Y_2 = Y_{12} + Y_{21} = b \sqcup\!\sqcup ab = bab + 2abb, \tag{18}$$

$$Y_1 \sqcup\!\sqcup Y_{21} = Y_{121} + 2Y_{211}, \tag{19}$$

and so on, from which we deduce

$$Y_{11} = W_{11},\ Y_{12} = W_{12} + W_{21},\ Y_{121} = W_{121} + W_{211}, \ldots \tag{20}$$

This leads to a triangular system of equations, which determines each Y_I as a linear combination with nonnegative integer coefficients of the W_J, such that $\ell(J) = \ell(I)$ and $J \geq I$ for the lexicographic order on compositions.

Here are the first transition matrices (entry (I, J) is the coefficient of W_I in Y_J). The indexation is the same all over the paper: the compositions are sorted according to the reverse lexicographic order. Note that zeroes have been replaced by dots to enhance readibility.

With $n = 4$, the indexations of the non-trivial blocks are respectively $(31), (22), (13)$ and $(211), (121), (112)$ and the matrices are

$$\begin{pmatrix} 1 & 2 & 1 \\ . & 1 & 1 \\ . & . & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 1 & 1 \\ . & 1 & 1 \\ . & . & 1 \end{pmatrix} \tag{21}$$

With $n = 5$, the indexations of the non-trivial blocks are respectively $(41), (32), (23), (14)$ and $(311), (221), (212), (131), (122), (113)$ and the matrices are

$$\begin{pmatrix} 1 & . & 6 & 1 \\ . & 1 & 2 & 1 \\ . & . & 1 & 1 \\ . & . & . & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & . & 6 & 1 & . & 1 \\ . & 1 & 1 & 1 & 2 & 1 \\ . & . & 1 & . & 1 & 1 \\ . & . & . & 1 & 2 & 1 \\ . & . & . & . & 1 & 1 \\ . & . & . & . & . & 1 \end{pmatrix} \tag{22}$$

One may observe the following properties of these matrices:

- They are triangular and block diagonal if compositions are ordered by reverse length-lexicographic order (e.g., $4, 31, 22, 13, 211, 121, 112, 1111$ for $n = 4$).
- The block for length k has therefore dimension $\binom{n-1}{k-1}$.

- Moreover, the sum of the entries of this block is the Stirling number of the second kind $S(n,k)$ (the number of set partitions of an n-set into k blocks.)

The first two properties are obvious. To prove the third one, define

$$P_{n,k} = \sum_{I\vDash n,\ \ell(I)=k} Y_I. \tag{23}$$

This can be rewritten as a sum over partitions

$$P_{n,k} = \sum_{\mu=(1^{m_1}2^{m_2}\cdots p^{m_p})\vdash n,\ \ell(\mu)=k} Y_{1^{m_1}} ⧢ Y_{2^{m_2}} ⧢ \cdots ⧢ Y_{p^{m_p}}, \tag{24}$$

and since

$$Y_{i^{m_i}} = \frac{W_i^{⧢ m_i}}{m_i!} \tag{25}$$

we see that $P_{n,k}$ is the coefficient of $x^n y^k$ in

$$\exp_{⧢}\left\{\sum_{m\ge 1} x^m y W_m\right\}. \tag{26}$$

Applying the character $W_n \mapsto 1/n!$ of $\mathbb{K}_{⧢}\langle a,b\rangle b$, we recognize the generating series of Stirling numbers of the second kind.

We shall now construct "better" matrices, sharing all these properties, and for which a closed formula can be given.

4. Dual approach

4.1. **Stalactic conguences and word-symmetric functions.** Alternatively, we can try to build a basis X_I of **Sym** whose coproduct is the binary unshuffle dual to the product of the Z_I. As above, we start with a basis V_I of **Sym** whose coproduct is dual to the shuffle of compositions. For example, we can take $V_I = X^I$, where X_n is a sequence of primitive generators. But there are other choices. For example, in [10], such a basis is obtained from a realization of **Sym** as a quotient of **WSym**, a Hopf algebra based on set partitions.

By definition, **WSym**(A) is the subspace of $\mathbb{K}\langle A\rangle$ spanned by the orbits of the symmetric group $\mathfrak{S}(A)$ acting on A^* by automorphisms. These orbits are naturally labelled by set partitions of $[n]$, the orbit corresponding to a partition π being constituted of the words

$$w = a_1 \dots a_n, \tag{27}$$

such that $a_i = a_j$ iff i and j are in the same block of π. The sum of these words will be denoted by $\mathbf{M}_\pi$.

For example,

$$\mathbf{M}_{\{\{1,3,6\},\{2\},\{4,5\}\}} := \sum_{a\neq b; b\neq c; a\neq c} abacca. \tag{28}$$

It is known that the natural coproduct of **WSym** (given as usual by the disjoint union of mutually commuting alphabets) is cocommutative [1] and that **WSym** is free over connected set partitions.

There are several ways to read an integer composition from a set partition. First, one can order the blocks according to the values of their minimal or maximal elements, and record the lenghts of the blocks. For example, we can order

$$\pi = \{\{3,4\},\{5\},\{1,2,6\}\} \tag{29}$$

in two ways, obtaining two set compositions

$$\Pi' = (126|34|5) \quad \text{and} \quad \Pi'' = (34|5|126) \tag{30}$$

and the integer compositions

$$K'(\pi) = (321) \quad \text{and} \quad K''(\pi) = (213)\,. \tag{31}$$

In [10], it is proved that the two-sided ideal of **WSym** generated by the differences $\mathbf{M}_\pi - \mathbf{M}_{\pi'}$ for $K'(\pi) = K'(\pi')$ is a Hopf ideal and that the quotient is isomorphic to **Sym**. This quotient can be interpreted in terms of a congruence on the free monoid A^*, the (left) *stalactic congruence*, introduced in [10]. It is generated by the relations

$$awa \equiv' aaw \quad \text{for } a \in A \text{ and } w \in A^*. \tag{32}$$

Thus, each word w is congruent to the word $P(w)$ obtained by moving each letter towards its leftmost occurence. Recording the original position of each letter by a set partition $Q(w)$, we obtain a bijection which is formally similar to (although much simpler than) the Robinson-Schensted correspondence, and **WSym** can be characterized as the costalactic algebra is the same way as **FSym** is the coplactic algebra [4]. One can of course also define a right stalactic congruence by

$$awa \equiv'' waa \quad \text{for } a \in A \text{ and } w \in A^*. \tag{33}$$

The same properties hold with the symmetric condition $K''(\pi) = K''(\pi')$, which amounts to take the right stalactic quotient. From now on, we write K instead of K'', and denote by V_I the equivalence class of $\mathbf{M}_\pi$ such that $K(\pi) = I$.

One can also record the values of the minimal and maximal elements of the blocks in the form of a composition. The minimal elements form a subset of $[n]$ always containing 1, so that we can decrement each of them and remove 0 so as to obtain a subset of $[n-1]$ which can be encoded by a composition $C'(\pi)$ of n. Similarly, the maximal elements form a subset always containing n, so that removing n, we obtain again a subset of $[n-1]$ and a composition $C''(\pi)$ of n. For example, with π as above,

$$C'(\pi) = (222) \quad \text{and} \quad C''(\pi) = (411)\,. \tag{34}$$

We shall choose the second option and write $C(\pi)$ for $C''(\pi)$.

Clearly, both $C(\pi)$ and $K(\pi)$ have the same length, which is the number of blocks of π.

4.2. **A sub-coalgebra of WSym.** Aside from being a quotient of **WSym**, **Sym** is also a sub coalgebra of **WQSym**. More precisely,

Theorem 4.1. *The sums*

$$\mathbf{X}_J = \sum_{C(\pi)=J} \mathbf{M}_\pi \tag{35}$$

span a sub-coalgebra of **WSym**, *and*

$$\Delta \mathbf{X}_J = \sum_{K,L} \langle W_J | W_K \sqcup\!\sqcup W_L \rangle \mathbf{X}_K \otimes \mathbf{X}_L \,. \tag{36}$$

Proof – This can be seen on an appropriate encoding.

Note first that the partitions of a set S of integers can be encoded by the set $\mathrm{SW}(S)$ of signed words whose letters are the elements of S, signed values appearing in increasing order of their absolute values, and such that $|w_i| < |w_{i+1}|$ if w_i is unsigned. Indeed, order the parts according to their maximal elements, sort each part in increasing order, read all parts successively and sign (overline) the last element of each part. For example,

$$\Pi = (346|5|127) \mapsto 34\overline{6}\overline{5}12\overline{7}. \tag{37}$$

Now, given a set S and a subset S', define $\mathrm{SP}(S, S')$ as the set of set partitions of S whose set of maximal elements of the parts is S'. For example, with $S = \{1, 3, 5, 6\}$ and $S' = \{3, 5, 6\}$, we have

$$\mathrm{SP}(S, S') = \{(13|5|6), (3|15|6), (3|5|16)\}. \tag{38}$$

Note that S and S' are unambiguously determined by the nondecreasing word $w(S, S')$ whose letters are the elements of S, with the elements of S' overlined. When applied to the signed permutation σ_I, the identity with the descents of I overlined, this process encodes the definition of $\mathbf{X}_I$ as a sum of $\mathbf{M}_\pi$.

Finally, given a set partition π, denote by $\mathrm{Co}(\pi)$ the set of pairs obtained by splitting the parts of π into two subsets in all possible ways. This encodes the coproduct of an $\mathbf{M}_\pi$ expressed in terms of tensor products $\mathbf{M}_{\pi'} \otimes \mathbf{M}_{\pi''}$.

To compute $\Delta\mathbf{X}_I$, we apply successively SP and Co to the signed word σ_I. We then obtain the set $S(I)$ of pairs of non-intersecting set partitions whose union is a set partition of $[1, n]$ and whose maximal elements of the blocks are exactly the descents of I.

We shall now check that we get the same result for the coproduct of a basis X_I of **Sym** dual to a basis Z_I of *QSym* whose product is given by (12). The coproduct of X_I can be computed by the following algorithm. Start with the signed permutation σ_I defined as above. It is clearly an encoding of the word W_I: an overlined letter corresponds to a b, and the other ones to an a. Thus, the coproduct of such a basis is encoded by the set of pairs of words (w_1, w_2) such that σ_I occurs in $w_1 \sqcup\!\sqcup w_2$, and such that w_1 and w_2 end by a signed letter. Now, to get this expression from $\Delta\mathbf{X}_I$ expanded as a linear combination of terms $\mathbf{M}_{\pi'} \otimes \mathbf{M}_{\pi''}$, one only needs to apply SP to each word w separately. This yields exactly the same set $S(I)$. Indeed, both sets are multiplicity-free; the second set is a subset of $S(I)$ since one can only obtain set partitions with given maximal values when applying SP; and the second set must contain $S(I)$, since any element of $S(I)$ gives back an unshuffling of σ_I when reordering its two subset partitions. ∎

Corollary 4.2. *For two compositions I and J of n, of the same length k, let*

$$c_{IJ} = \#\{\pi \in \Pi_n \mid K(\pi) = I \text{ and } C(\pi) = J\}, \quad \text{and } X_J = \sum_I c_{IJ} V_I \,. \tag{39}$$

Then, the dual basis Z_I of X_I satisfies the binary shuffle product rule (12).

Proof – Denoting by $\bar{\mathbf{M}}_\pi$ the stalactic class of $\mathbf{M}_\pi$, we have by definition

$$X_J = \sum_{C(\pi)=J} \bar{\mathbf{M}}_\pi \,. \tag{40}$$

Since the canonical projection $p: \mathbf{M}_\pi \mapsto \bar{\mathbf{M}}_\pi$ is a Hopf algebra morphism, we have

$$\Delta X_J = \sum_{K,L} \langle W_J | W_K \sqcup\!\sqcup W_L \rangle X_K \otimes X_L \,. \tag{41}$$

■

Example 4.3. Let us compute $\Delta(\mathbf{X}_{221})$. By definition,

$$\mathbf{X}_{211} = \mathbf{M}_{12|3|4} + \mathbf{M}_{2|13|4} + \mathbf{M}_{2|3|14}, \tag{42}$$

which can be encoded as

$$1\overline{234} + \bar{2}1\overline{34} + \overline{23}1\bar{4}. \tag{43}$$

Extracting subwords ending by a signed letter yields the following list $S(211)$ of pairs of words:

$$\begin{array}{c} (1\overline{23}, \bar{4}), (1\overline{24}, \bar{3}), (1\bar{2}, \overline{34}) \\ (\bar{2}1\bar{3}, \bar{4}), (1\overline{34}, \bar{2}), (1\bar{3}, \overline{24}) \\ (\bar{2}1\bar{4}, \bar{3}), (\bar{3}1\bar{4}, \bar{2}), (1\bar{4}, \overline{23}) \end{array} \tag{44}$$

together with the symmetrical pairs, where 1 then belongs to the right part. The theorem states that $\Delta\mathbf{X}_{211}$ can be computed by the unshuffling of the word $1\overline{234}$, which gives the set of words

$$\begin{array}{c} (1\overline{23}, \bar{4}), (1\overline{24}, \bar{3}), (1\overline{34}, \bar{2}) \\ (1\bar{2}, \overline{34}), (1\bar{3}, \overline{24}), (1\bar{4}, \overline{23}) \end{array} \tag{45}$$

and their symmetrical pairs, where 1 occurs on the right. The words in these pairs can now be decoded into lists of sets partitions according to the remark following Eq. (38). This gives the set of Equation (44): the first three words give rise to two pairs of partitions (the first one gives both $(1\overline{23}, \bar{4})$ and $(\bar{2}1\bar{3}, \bar{4})$) whereas the last three ones yield only one.

Since we have only used the coproduct rule of the basis V_I, we have as well:

Corollary 4.4. *The same is true if one replaces V_I by any basis whose coproduct is the unshuffle of compositions, for example a basis of product of primitive elements such as Ψ^I or Φ^I.*

4.3. **Generating functions and closed formulas.**

Proposition 4.5. *For two compositions I, J of n of the same length k,*

$$c_{IJ} = \prod_{s=1}^{k} \binom{j_1 + \cdots + j_s - (i_1 + \cdots + i_{s-1}) - 1}{i_s - 1}. \tag{46}$$

Examples of the matrices $C = (c_{IJ})$ are given in Section 5.

Proof – Let π be a set partition such that $C(\pi) = J$, and order the blocks by increasing maxima. The first block is composed of j_1 and of $i_1 - 1$ elements strictly smaller than j_1, which yields $\binom{j_1-1}{i_1-1}$ choices. Having chosen those elements, the second block is composed of $j_1 + j_2$, and of $i_2 - 1$ elements smaller than $j_1 + j_2$, and different from the i_1 elements of the first block, which leaves us with $\binom{j_1+j_2-1-i_1}{i_2-1}$ choices, and so on. ■

These expressions have simple generating series, which allow to find immediately the inverse matrices.

Proposition 4.6. *For a composition J of n of length k, the generating function of the column c_{IJ} is*

$$\sum_{I\vDash n,\ \ell(I)=k} c_{IJ} \prod_{s=1}^{k} x_s^{i_s-1} = \prod_{s=1}^{k} (x_s + \cdots + x_k)^{j_s-1} . \tag{47}$$

Corollary 4.7. *Let Z_J be the dual basis of X_J, and U_I be the dual basis of V_I in QSym. Set*

$$Z_I = \sum_J d_{IJ} U_J , \tag{48}$$

where D is the transpose of C^{-1}. The generating function of row I is

$$\sum_J d_{IJ} \prod_{s=1}^{k} y_s^{j_s-1} = \prod_{s=1}^{k} (y_s - y_{s+1})^{j_s-1} \quad (\textit{with } y_{k+1} := 0) \tag{49}$$

Proof – Define $y_i = x_i + \cdots + x_k$. Then the system of equations

$$y_1^{j_1-1} y_2^{j_2-1} \cdots y_k^{j_k-1} = (x_1 + \cdots + x_k)^{j_1-1} (x_2 + \cdots + x_k)^{j_2-1} \cdots x_k^{j_k-1} \tag{50}$$

for all compositions of n of length k is clearly equivalent to

$$x_k = y_k, \quad x_{k-1} = y_{k-1} - y_k, \quad \ldots, \quad x_1 = y_1 - y_2 . \tag{51}$$

■

For example, we can read on the matrices below that

$$X_{12} = V_{12},\ X_{21} = V_{21} + V_{12},\ \text{so that } Z_{21} = U_{21} \text{ and } Z_{12} = U_{12} - U_{21}. \tag{52}$$

Hence, since $U_I U_J$ is given by the shuffle of compositions,

$$Z_1 Z_{21} = 2U_{211} + U_{121} = Z_{121} + 3Z_{211} \tag{53}$$

and

$$Z_1 Z_{12} = 2U_{211} - 2U_{211} = 2Z_{112} + 2Z_{121} \tag{54}$$

as one can read $U_{211} = Z_{221}$, $U_{121} = Z_{121} + Z_{211}$ and $U_{112} = Z_{112} + Z_{121} + Z_{211}$.

4.4. **Relations with Ecalle's generating functions.** By Corollary 4.4, we can assume that $V_I = Y^I$, where $Y^I = Y_{i_1} \cdots Y_{i_r}$ is the multiplicative basis of **Sym** constructed from a generating sequence (Y_n) of the primitive Lie algebra of **Sym**. Let U_I be the dual basis of Y^I in *QSym*. Then, by Corollary 4.7, we have

$$\sum_{\ell(J)=k} Z_J y_1^{j_1-1} y_2^{j_2-1} \cdots y_k^{j_k-1} = \sum_{\ell(I)=k} U_I x_1^{i_1-1} x_2^{i_2-1} \cdots x_k^{i_k-1}\,. \tag{55}$$

A similar relation (up to reversal of the indices) occurs in Ecalle's works on MZVs. If in the l.h.s. we replace Z_J by the integral representation (10) of $\zeta(J)$ (denoted by Wa^J in [5]), the l.h.s. becomes what Ecalle denotes by $\mathrm{Zag}^{(x_1,\dots,x_k)}$ (actually, Ecalle works with colored MZVs and there is a second set of parameters). The equality (55) translates into the statement "$\mathrm{Wa}^\bullet$ symmetral $\Leftrightarrow$ $\mathrm{Zag}^\bullet$ symmetral". Indeed, by definition, the symmetrality of $\mathrm{Wa}^\bullet$ is equivalent to the product formula

$$U_I U_J = \sum_K \langle K \mid I \sqcup\!\sqcup J\rangle U_K\,, \tag{56}$$

which, written in the form of a generating function, reads

$$\mathrm{Zag}^{(x_1,\dots,x_k)}\mathrm{Zag}^{(x_{k+1},\dots,x_n)} = \sum_{\sigma\in 12\cdots k \sqcup\!\sqcup k+1\cdots n} \mathrm{Zag}^{\left(x_{\sigma^{-1}(1)},\dots,x_{\sigma^{-1}(n)}\right)}. \tag{57}$$

4.5. **Noncommutative Bell polynomials.** To be more specific, one may take the multiplicative basis Y^I constructed from the normalized Dynkin elements $Y_n = (n-1)!\Psi_n$. Then,

$$\sum_{J\vDash n} X_J = \sum_{I\vDash n} \beta_I Y^I = B_n(Y) \tag{58}$$

is the noncommutative Bell polynomial in the Y_i as defined in [19] by the recursive formula

$$B_{n+1} = \sum_{k=0}^{n} \binom{n}{k} B_{n-k} Y_{k+1} \quad \text{and} \quad B_0 = 1 \tag{59}$$

which translates into the recursion

$$(n+1)S_{n+1} = \sum_{k=0}^{n} S_{n-k}\Psi_{k+1} \tag{60}$$

after the change of variables, so that for this choice of the Y_i, it reduces to $n!S_n$.

4.6. **Direct construction from binary words.** Rather surprisingly, the coefficients c_{IJ}, which have been obtained in a canonical way from **WSym** without choosing a basis of **Sym**, can also be obtained by a very specific choice, the above normalized version of the Ψ basis, interpreted in terms of Lie polynomials in two letters.

Dual to the realization of *QSym* as a subalgebra of $\mathbb{K}_{\sqcup\!\sqcup}\langle a, b\rangle$, there is a simple realization of **Sym** as a subalgebra of $\mathbb{K}\langle a, b\rangle$, regarded as the universal enveloping algebra of $L(a, b)$, the free Lie algebra on two letters. If one sets

$$\Psi_n = \frac{1}{(n-1)!}\mathrm{ad}_a^{n-1} b = \frac{1}{(n-1)!}[a,[a,[\dots,[a,b]\dots]]] \tag{61}$$

then there is a simple expression for S_n:

$$S_n = \frac{1}{n!}\sum_{k=0}^{n}\binom{n}{k}(-1)^k(a+b)^{n-k}a^k\,. \tag{62}$$

Indeed,

$$\psi(t) := \sum_{n\geq 1} t^{n-1}\Psi_n = e^{t\,\mathrm{ad}_a}b = e^{ta}be^{-ta} \tag{63}$$

so that the differential equation for $x(t)=\sum_n t^nS_n$, which is

$$x'(t) = x(t)\psi(t) \quad \text{with } x(0)=1 \tag{64}$$

yields

$$x(t) = e^{t(a+b)}e^{-ta}\,. \tag{65}$$

The algebra morphism defined by $\iota\,:\,(n-1)!\Psi_n \mapsto Y_n = \mathrm{ad}_a^{n-1}b$ is also a coalgebra morphism, as it sends primitive elements to primitive elements. However, since the Z-bases define embeddings of $QSym$ as a subalgebra of $\mathbb{K}_{\sqcup\!\sqcup}\langle a,b\rangle b$, by duality, **Sym** should be a quotient coalgebra of $\mathbb{K}\langle a,b\rangle b$.

Let $\mathfrak{p}:\ \mathbb{K}\langle a,b\rangle\to\mathbb{K}\langle a,b\rangle b$ be the projection defined by $\mathfrak{p}(w)=0$ if w ends by a, and let

$$\Delta' = (\mathfrak{p}\otimes\mathfrak{p})\circ\Delta \tag{66}$$

where Δ is the usual coproduct of $\mathbb{K}\langle a,b\rangle$ (for which the letters are primitive). Then,

$$\mathfrak{p}(Y_n) = a^{n-1}b = W_n \tag{67}$$

is primitive for Δ'. For $I=(i_1,\dots,i_r)$,

$$\mathfrak{p}(Y^I) = Y^{i_1,\dots,i_{r-1}}\mathfrak{p}(Y_{i_r}) \tag{68}$$

and by induction on r,

$$\Delta'\circ\mathfrak{p}(Y^I) = (\mathfrak{p}\otimes\mathfrak{p})\circ\Delta(Y^I) \tag{69}$$

so that $\mathfrak{p}$ induces an isomorphism of coalgebras

$$\mathfrak{p}:\ (\iota(\mathbf{Sym}),\Delta)\longrightarrow(\mathbb{K}\langle a,b\rangle b,\Delta')\,. \tag{70}$$

Now,

$$Y_n = \sum_{k=0}^{n-1}(-1)^k\binom{n-1}{k}a^{n-1-k}ba^k \tag{71}$$

and a straightforward calculation (see [16, Appendix A]) shows that

$$\mathfrak{p}(Y^I) = \sum_J d_{IJ}W_J \tag{72}$$

where the d_{IJ} are as in Corollary 4.7. By duality, the image Z_I in $QSym$ of the dual basis W_I^* by $\iota^*\circ\mathfrak{p}^*$ satisfies the binary shuffle relations (12). These considerations, which are essentially in Racinet's thesis [16] explain the appearance of the generating functions (49) and (47) in the theory of MZVs, and in particular Ecalle's swap operation. We can now see that they follow from a particular choice of a generating sequence of the primitive Lie algebra of **Sym**, together with a specific embedding of **Sym** in $\mathbb{K}\langle a, b\rangle$.

Finally, it is instructive to play a little with the noncommutative Bell polynomials in this context. Setting $Y_k = \mathrm{ad}_a^{k-1} b$ in the noncommutative Bell polynomials, this yields

$$B_n = \sum_{k=0}^{n} \binom{n}{k} (-1)^k (a+b)^{n-k} a^k \,. \tag{73}$$

Let now L be the linear operator

$$L = \mathrm{ad}_a + b\,. \tag{74}$$

Let D denote the derivation ad_a, and set $b^{(k)} = D^k b$. According to [19, Theorem 2],

$$B_n(b, b', b'', \dots, b^{(n-1)}) = L^n(1). \tag{75}$$

Thus, the above considerations amount to that fact $L^n(1)$ is equal to the r.h.s of (73), which can of course be proved directly:

$$x(t) := e^{t(a+b)} e^{-ta} \tag{76}$$

satisfies obviously

$$\frac{dx}{dt} = (a+b)x - xa = Lx, \quad x(0) = 1\,. \tag{77}$$

Comparing (47) with [19, Theorem 2], we obtain the binomial identity

Corollary 4.8. *The column sums of the matrices (c_{IJ}) are*

$$\sum_{J \vDash n,\ \ell(J)=k} \prod_{s=1}^{k} \binom{j_1 + \cdots + j_s - (i_1 + \cdots + i_{s-1}) - 1}{i_s - 1} = \prod_{s=2}^{k} \binom{i_1 + \cdots + i_s - 1}{i_1 + \cdots + i_{s-1}}. \tag{78}$$

5. Matrices

The entry in row I and column J is the coefficient of V_I in X_J in the first matrix, and the coefficient of U_I in Z_J in the second one.

Case $n = 3$, $k = 2$

$$\begin{pmatrix} 1 & . \\ 1 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & -1 \\ . & 1 \end{pmatrix} \tag{79}$$

Case $n = 4$ with $k = 2$ and $k = 3$.

$$\begin{pmatrix} 1 & . & . \\ 2 & 1 & . \\ 1 & 1 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & -2 & 1 \\ . & 1 & -1 \\ . & . & 1 \end{pmatrix} \tag{80}$$

$$\begin{pmatrix} 1 & . & . \\ 1 & 1 & . \\ 1 & 1 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & -1 & . \\ . & 1 & -1 \\ . & . & 1 \end{pmatrix} \tag{81}$$

Case $n = 5$, for all values of k from 2 to 4.

$$\begin{pmatrix} 1 & . & . & . \\ 3 & 1 & . & . \\ 3 & 2 & 1 & . \\ 1 & 1 & 1 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & -3 & 3 & -1 \\ . & 1 & -2 & 1 \\ . & . & 1 & -1 \\ . & . & . & 1 \end{pmatrix} \tag{82}$$

$$\begin{pmatrix} 1 & . & . & . & . & . \\ 2 & 1 & . & . & . & . \\ 2 & 1 & 1 & . & . & . \\ 1 & 1 & . & 1 & . & . \\ 2 & 2 & 1 & 2 & 1 & . \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & -2 & . & 1 & . & . \\ . & 1 & -1 & -1 & 1 & . \\ . & . & 1 & . & -1 & . \\ . & . & . & 1 & -2 & 1 \\ . & . & . & . & 1 & -1 \\ . & . & . & . & . & 1 \end{pmatrix} \tag{83}$$

$$\begin{pmatrix} 1 & . & . & . \\ 1 & 1 & . & . \\ 1 & 1 & 1 & . \\ 1 & 1 & 1 & 1 \end{pmatrix} \qquad \begin{pmatrix} 1 & -1 & . & . \\ . & 1 & -1 & . \\ . & . & 1 & -1 \\ . & . & . & 1 \end{pmatrix} \tag{84}$$

For $k = 2$, the block is always given by the Pascal triangle. For $k = n - 1$, it is the lower triangular matrix with all entries equal to 1. Here follows the remaining blocks for $n = 6$, that is, for $k = 3$ and 4.

$$\begin{pmatrix} 1 & . & . & . & . & . & . & . & . & . \\ 3 & 1 & . & . & . & . & . & . & . & . \\ 3 & 1 & 1 & . & . & . & . & . & . & . \\ 3 & 2 & . & 1 & . & . & . & . & . & . \\ 6 & 4 & 2 & 2 & 1 & . & . & . & . & . \\ 3 & 2 & 2 & 1 & 1 & 1 & . & . & . & . \\ 1 & 1 & . & 1 & . & . & 1 & . & . & . \\ 3 & 3 & 1 & 3 & 1 & . & 3 & 1 & . & . \\ 3 & 3 & 2 & 3 & 2 & 1 & 3 & 2 & 1 & . \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & -3 & . & 3 & . & . & -1 & . & . & . \\ . & 1 & -1 & -2 & 2 & . & 1 & -1 & . & . \\ . & . & 1 & . & -2 & . & . & 1 & . & . \\ . & . & . & 1 & -2 & 1 & -1 & 2 & -1 & . \\ . & . & . & . & 1 & -1 & . & -1 & 1 & . \\ . & . & . & . & . & 1 & . & . & -1 & . \\ . & . & . & . & . & . & 1 & -3 & 3 & -1 \\ . & . & . & . & . & . & . & 1 & -2 & 1 \\ . & . & . & . & . & . & . & . & 1 & -1 \\ . & . & . & . & . & . & . & . & . & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & . & . & . & . & . & . & . & . & . \\ 2 & 1 & . & . & . & . & . & . & . & . \\ 2 & 1 & 1 & . & . & . & . & . & . & . \\ 2 & 1 & 1 & 1 & . & . & . & . & . & . \\ 1 & 1 & . & . & 1 & . & . & . & . & . \\ 2 & 2 & 1 & . & 2 & 1 & . & . & . & . \\ 2 & 2 & 1 & 1 & 2 & 1 & 1 & . & . & . \\ 1 & 1 & 1 & . & 1 & 1 & . & 1 & . & . \\ 2 & 2 & 2 & 1 & 2 & 2 & 1 & 2 & 1 & . \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & -2 & . & . & 1 & . & . & . & . & . \\ . & 1 & -1 & . & -1 & 1 & . & . & . & . \\ . & . & 1 & -1 & . & -1 & 1 & . & . & . \\ . & . & . & 1 & . & . & -1 & . & . & . \\ . & . & . & . & 1 & -2 & . & 1 & . & . \\ . & . & . & . & . & 1 & -1 & -1 & 1 & . \\ . & . & . & . & . & . & 1 & . & -1 & . \\ . & . & . & . & . & . & . & 1 & -2 & 1 \\ . & . & . & . & . & . & . & . & 1 & -1 \\ . & . & . & . & . & . & . & . & . & 1 \end{pmatrix}$$

Comparing these matrices with the matrices given in Equations (21) and (22), on sees that the transposes of the matrices giving the coefficient of Z_I on U_J has many similarities with those constructed by the recursive procedure of Section3.

6. Rational functions and colored free quasi-symmetric functions

Recall that *QSym* is the commutative image of the algebra **FQSym** of free quasi-symmetric functions, that is, $F_I(X)$ is obtained by sending the noncommutating variables a_i of

$$\mathbf{F}_\sigma(A) = \sum_{\mathrm{std}(w)=\sigma^{-1}} w \tag{85}$$

to commuting variables x_i.

In [3], the vector space **FQSym** is identified to the Zinbiel operad, realized as a suboperad of the operad of rational moulds.

A *mould*, as defined by Ecalle, is a "function of a variable number of variables", that is, a sequence $f = (f_n(u_1, \dots, u_n))$ of functions of n (continuous or discrete) variables. There is a bilinear operation defined componentwise by

$$\mathrm{mu}(f_n, g_m) = f_n(u_1, \dots, u_n) g_m(u_{n+1}, \dots, u_{n+m}) \tag{86}$$

which defines an associative product $*$ on homogeneous moulds (those with only one f_n nonzero). For this product, the rational functions

$$f_\sigma(u_1, \dots, u_n) = \frac{1}{u_{\sigma(1)}(u_{\sigma(1)} + u_{\sigma(2)}) \cdots (u_{\sigma(1)} + u_{\sigma(2)} + \cdots + u_{\sigma(n)})} \tag{87}$$

span a subalgebra isomorphic to **FQSym** under the correspondence $f_\sigma \mapsto \mathbf{F}_\sigma$.

In [8], it is proved that the fractions

$$z_{\sigma,s}(u_1, \dots, u_n) = \frac{1}{u_{\sigma(1)}^{s_1}(u_{\sigma(1)} + u_{\sigma(2)})^{s_2} \cdots (u_{\sigma(1)} + u_{\sigma(2)} + \cdots + u_{\sigma(n)})^{s_n}} \tag{88}$$

where $\sigma \in \mathfrak{S}_n$ and $s \in \mathbb{N}^{*n}$ satisfy a product formula generalizing the binary shuffle (12). That is, if one sets

$$\epsilon_{\sigma,s} = 0^{s_1-1}\sigma_1 0^{s_2-1}\sigma_2 \cdots 0^{s_n-1}\sigma_n \tag{89}$$

then,

$$z_{\sigma,s} * z_{\tau,t} = \sum_{\omega,w} \langle \epsilon_{\omega,w} | \epsilon_{\sigma,s} \sqcup\!\sqcup\, \epsilon_{\tau[n],t} \rangle z_{\omega,w} \tag{90}$$

where $\tau[n]$ denotes as usual the permutation τ shifted by the length of $\sigma \in \mathfrak{S}_n$. There is a natural bigrading $\deg z_{\sigma,s} = (n, |s|)$ if $\sigma \in \mathfrak{S}_n$ and $|s| = \sum s_i$.

Again, there exist colored versions of **FQSym**, based on symbols $\mathbf{F}_{\sigma,c}$ where $\sigma \in \mathfrak{S}_n$ and $c \in C^n$ is a color word, C being the color alphabet. Taking $C = \mathbb{N}^*$, we obtain a bigraded vector space isomorphic to the linear span of the $z_{\sigma,s}$. The product rule is

$$\mathbf{F}_{\sigma',c'} \mathbf{F}_{\sigma'',c''} = \sum_{(\sigma,c) \in (\sigma',c') \Cup (\sigma'',c'')} \mathbf{F}_{\sigma,c}\,, \tag{91}$$

where the shifted shuffle $\Cup$ of colored permutations is computed by shifting the letters of σ'' by the size of σ' and shuffling the colored letters.

Thus, $\mathbf{F}_{\sigma,s} \mapsto z_{\sigma,s}$ is not an isomorphism of algebras, but the previous considerations allow us to prove:

Theorem 6.1. *Define a basis* $\mathbf{Z}_{\sigma,J}$ *by*

$$\mathbf{F}_{\sigma,I} = \sum_{|J|=|I|} c_{IJ} \mathbf{Z}_{\sigma,J} \tag{92}$$

for $\sigma \in \mathfrak{S}_n$ *and* I *a composition of length* n*, the* c_{IJ} *being as in* (47)*. Then,*

$$\mathbf{Z}_{\sigma',J'} \mathbf{Z}_{\sigma'',J''} = \sum_{\sigma,J} \langle \epsilon_{\sigma,J} | \epsilon_{\sigma',I'} ⧢ \epsilon_{\sigma''[n],I''} \rangle \mathbf{Z}_{\sigma,J}. \tag{93}$$

Proof – This can be seen, for example, by a straightforward generalization of the argument of Section 4.6. Replace the letter b by an alphabet $B = \{b_i | i \geq 1\}$, and define elements of $\mathbb{K}\langle a, B\rangle$ by

$$Y^{i,n} = \mathrm{ad}_a^{n-1} b_i, \quad Y^{u,I} = Y^{u_1,i_1} \cdots Y^{u_r,i_r} \tag{94}$$

for a word $u = u_1 \cdots u_r$ and a composition $I = (i_1, \ldots, i_r)$.

Let, as before $\mathfrak{p} : \mathbb{K}\langle a, B\rangle \to \bigoplus_{b\in B} \mathbb{K}\langle a, B\rangle b$ be the projection defined by $\mathfrak{p}(w) = 0$ if w ends by a, and

$$\Delta' = (\mathfrak{p} \otimes \mathfrak{p}) \circ \Delta \tag{95}$$

where Δ is the usual coproduct of $\mathbb{K}\langle a, B\rangle$ for which the letters are primitive. Then,

$$\mathfrak{p}(Y^{i,n}) = a^{n-1} b_i =: W_{i,n} \tag{96}$$

is primitive for Δ', and

$$\mathfrak{p}(Y^{u,I}) = Y^{u_1,i_1} \cdots Y^{u_{r-1},i_{r-1}} \mathfrak{p}(Y^{u_r,i_r}) \tag{97}$$

so that

$$\Delta' \circ \mathfrak{p}(Y^{u,I}) = (\mathfrak{p} \otimes \mathfrak{p}) \circ \Delta(Y^{u,I}) \tag{98}$$

Assuming now that $u = \sigma$ is a permutation, and taking into account the product rule of $\mathbf{FQSym}^{(\mathbb{N}^*)}$, we can also write this coproduct in the form

$$\Delta' \circ \mathfrak{p}(Y^{u,I}) = \sum_{u',I';u'',I''} \langle \mathbf{F}_{\sigma,I} | \mathbf{F}_{\mathrm{std}(u'),I'} \mathbf{F}_{\mathrm{std}(u''),I''} \rangle Y^{u',I'} \otimes Y^{u'',I''}. \tag{99}$$

Again,

$$\mathfrak{p}(Y^{\sigma,I}) = \sum_J d_{IJ} W_{\sigma,J}, \tag{100}$$

and the result follows from (99) by duality. ■

Taking into account the generating functions of Section 4.3, we have

$$\sum_{\ell(I)=n} y_1^{i_1-1} y_2^{i_2-1} \cdots y_n^{i_n-1} \mathbf{Z}_{\sigma,I} = \sum_{\ell(I)=n} (y_1 - y_2)^{i_1-1} (y_2 - y_3)^{i_2-1} \cdots y_n^{i_n-1} \mathbf{F}_{\sigma,I}. \tag{101}$$

Finally, it can be shown that the vector space spanned by the $z_{\sigma,I}$ is stable under the operadic compositions of [3]. The resulting operad will be investigated in a separate paper.

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