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ABSTRACT. We investigate deformations of the shuffle Hopf algebra structure Sh(A) which can be defined on the tensor algebra over a commutative algebra A. Such deformations, leading for example to the quasi-shuffle algebra QSh(A), can be interpreted as natural transformations of the functor Sh, regarded as a functor from commutative nonunital algebras to coalgebras. We prove that the monoid of natural endomophisms of the functor Sh is isomorphic to the monoid of formal power series in one variable without constant term under composition, so that in particular, its natural automorphisms are in bijection with formal diffeomorphisms of the line.

These transformations can be interpreted as elements of the Hopf algebra of word quasi-symmetric functions**WQSym**, and in turn define deformations of its struture. This leads to a new embedding of free quasi-symmetric functions into **WQSym**, whose relevance is illustrated by a simple and transparent proof of Goldberg's formula for the coefficients of the Hausdorff series.

INTRODUCTION

The tensor algebra over a commutative algebra A is provided by the shuffle product with a commutative (Hopf) algebra structure. However, other products (resp. Hopf algebra) structures can be defined, the best known one being the quasi-shuffle product (resp. quasi-shuffle Hopf algebra). These products arise in many contexts, *e.g.*, Rota–Baxter algebras, multiple zeta values (MZVs), noncommutative symmetric functions, operads ... Moreover, they are natural: they commute with morphisms of commutative algebras; in other terms, they define functors from the category of commutative algebras to that of commutative Hopf algebras.

The present paper aims at studying and classifying these products and Hopf algebra structures. The Faà di Bruno Hopf algebra plays a key role in this classification: its characters (in bijection with formal diffeomorphisms tangent to the identity) happen to classify the natural deformations of shuffle algebras considered in this article.

Our approach also sheds a new light on classical constructions such as quasi-shuffles. Most structure properties of quasi-shuffle algebras appear, from our point of view, as straightforward consequences of their definition as deformations by conjugacy of shuffle algebras. This allows to transport automatically *all* known results on shuffle algebras to quasi-shuffles and does not require the algebra A to be graded (compare, *e.g.*, [11]). We may quote the existence of a "natural" (but not straightforward !) gradation, and of fine Hopf algebraic properties such as the ones studied in [14].

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Most of these results can be phrased in terms of combinatorial properties of Hopf algebras based on permutations (free quasi-symmetric functions) and surjections (word quasi-symmetric functions). In particular, the analysis of the relations between shuffles and quasi-shuffles leads to a new polynomial realization of noncommutative symmetric functions, which can be extended to free quasi-symmetric functions. Beyond its naturallity from the point of view of quasi-shuffle algebras, this new realization has an interest on its own: as an application, a simple (and, in our opinion, enlightening) proof of Goldberg's formula for the coefficients of the Haudorff series and a generalization thereof to other, similar, series is obtained.

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1. The shuffle algebra over a commutative algebra

Let A be a commutative algebra over the rationals[1], (not necessarily with a unit) and let $T(A)$ be its tensor algebra

$$T(A) = \bigoplus_{n\in\mathbb{N}} T_n(A) = \bigoplus_{n\in\mathbb{N}} A^{\otimes n}$$

with $A^{\otimes 0} := \mathbf{Q}$. Tensors $a_1 \otimes ... \otimes a_n$ in $T_n(A)$ will be written as words $a_1...a_n$, the $\otimes$ sign being reserved for tensor products of elements of $T(A)$.

The concatenation product in $T(A)$ is written $\times$ to distinguish it from the internal product in A

$$a_1...a_n \times b_1...b_m := a_1...a_n b_1...b_m.$$

The (internal) product of a and b in A will be always written $a \cdot b \in A$ (and not ab, which represents an element in $A^{\otimes 2}$).

Definition 1. *The shuffle bialgebra* $\mathrm{Sh}(A) = \bigoplus_{n\in\mathbb{N}} \mathrm{Sh}_n(A)$ *is the graded connected (i.e.* $\mathrm{Sh}_0(A) = \mathbf{Q}$*) commutative Hopf algebra such that*

- *As vector spaces* $\mathrm{Sh}_n(A) = T_n(A)$.
- *Its product* $\sqcup\!\sqcup$ *is defined recursively as the sum of the two half-shuffle products* $\prec$, $\succ$

$$a_1...a_n \prec b_1...b_p := a_1 \times (a_2...a_n \sqcup\!\sqcup\, b_1...b_p)$$

$$a_1...a_n \succ b_1...b_p := b_1...b_p \prec a_1...a_n = b_1 \times (a_1...a_n \sqcup\!\sqcup\, b_2...b_p),$$

  and $\sqcup\!\sqcup = \prec + \succ$.
- *Its coalgebra structure is defined by the deconcatenation coproduct*

$$\Delta(a_1...a_n) := \sum_{0\le k\le n} a_1...a_k \otimes a_{k+1}...a_n.$$

[1]Any field of characteristic zero would be suitable as well.

Recall that the notions of connected commutative Hopf algebra and connected commutative bialgebra are equivalent since a graded connected commutative bialgebra always has an antipode [13].

The above construction is functorial: $\mathrm{Sh} : A \to \mathrm{Sh}(A)$ is a functor from the category of commutative algebras without a unit to the category of graded connected commutative Hopf algebras. Since a vector space can be viewed as a commutative algebra with the null product, our definition of $\mathrm{Sh}(A)$ encompasses the contruction of the shuffle algebra over a vector space. Although it may seem artificial at the moment (since we did not make use of the internal product $\cdot$ to define $\mathrm{Sh}(A)$), viewing Sh as a functor from commutative algebras to graded connected commutative Hopf algebras is better suited to the forthcoming developments.

Equivalently, for all $a_1, \dots, a_{k+l} \in A$,

$$\begin{aligned} a_1 \dots a_k \prec a_{k+1} \dots a_{k+l} &= \sum_{\alpha \in \mathrm{Des}_{\subseteq \{k\}},\, \alpha^{-1}(1)=1} a_{\alpha^{-1}(1)} \dots a_{\alpha^{-1}(k+l)}, \\ a_1 \dots a_k \succ a_{k+1} \dots a_{k+l} &= \sum_{\alpha \in \mathrm{Des}_{\subseteq \{k\}},\, \alpha^{-1}(1)=k+1} a_{\alpha^{-1}(1)} \dots a_{\alpha^{-1}(k+l)}, \end{aligned}$$

where the α are permutations of $[k+l] = \{1, ..., k+l\}$.

The notation $\alpha \in \mathrm{Des}_{\subseteq \{k\}}$ means that α has at most one descent in position k. Recall that a permutation σ of $[n]$ is said to have a descent in position $i < n$ if $\sigma(i) > \sigma(i+1)$. The descent set of σ, $desc(\alpha)$ is the set of all descents of α,

$$desc(\sigma) := \{i < n, \sigma(i) > \sigma(i+1)\}.$$

For $I \subset [n]$, we write $\mathrm{Des}_I := \{\sigma, \mathrm{desc}(\sigma) = I\}$ and $\mathrm{Des}_{\subseteq I} := \{\sigma, \mathrm{desc}(\sigma) \subseteq I\}$.

A Theorem due to Schützenberger [20] characterizes abstractly the shuffle algebras:

Proposition 2. *As a commutative algebra,* $\mathrm{Sh}(A)$ *is the free algebra* over the vector space A for the relation

$$(a \prec b) \prec c = a \prec (b \prec c + c \prec b). \tag{1}$$

An algebra equipped with a product $\prec$ satisfying this relation is sometimes refered to as a chronological algebra (although the term has also other meanings) or as a Zinbiel algebra (because it is dual to Cuvier's notion of Leibniz algebra), we refer to [6] for historical details.

A last ingredient of the theory of tensors and shuffle algebras over commutative algebras will be useful: namely, the nonlinear Schur-Weyl duality established in [14]. Let us recall that **WQSym** stands for the Hopf algebra of word quasi-symmetric functions. This algebra can be given various equivalent realizations (that is, its elements can be encoded by means of surjections, packed words, set compositions or faces of permutohedra) and carries various algebraic structures on which we will come back later. We refer, *e.g.*, to [14] for details. It will appear later in this article that, whereas the realization of **WQSym** in terms of surjections is the one suited for studying deformations of shuffle algebras, that in terms of words is the one suited to the analysis of Hausdorff series.

For the time being, we simply recall that **WQSym** can be realized as the linear span of all surjections f from $[n]$ to $[p]$, where n runs over the integers and $1 \leq p \leq n$ and postpone the definition of the product and the coproduct. We say that such a map f is of degree n, relative degree $n-p$, and bidegree (n,p). The linear span of degree n (resp. bidegree (n,p)) elements is written $\mathbf{WQSym}_n$ (resp. $\mathbf{WQSym}_{n,p}$). We write $\widehat{\mathbf{WQSym}}$ for $\prod\limits_{n,p} \mathbf{WQSym}_{n,p}$.

We consider now natural endomorphisms of the functor T, viewed as a functor from nonunital commutative algebras to vector spaces. Concretely, we look for families of linear maps μ_A from $T_n(A)$ to $T_m(A)$ (where A runs over nonunital commutative algebras and m and n run over the nonzero integers) such that, for any map f of nonunital commutative algebras from A to B,

$$T_m(f) \circ \mu_A = \mu_B \circ T_n(f). \tag{2}$$

Let us say that such a family μ_A satisfies the nonlinear Schur-Weyl duality (with parameters n, m). We have [14]:

Proposition 3. *The vector space of linear maps that satisfy the nonlinear Schur-Weyl duality with parameters n, m is canonically isomorphic to $\mathbf{WQSym}_{n,m}$, the linear span of surjections from $[n]$ to $[m]$. Equivalently, the vector space of natural endomorphisms of the functor T is canonically isomorphic to $\widehat{\mathbf{WQSym}}$.*

2. Natural coalgebra endomorphisms

The nonlinear Schur-Weyl duality shows that $\widehat{\mathbf{WQSym}}$ is the natural object for investigating the linear structure of the tensor and shuffle algebras over a commutative algebra. In this section and the following ones, we study shuffle algebras from a refined point of view. Namely, we aim at characterizing, inside $\widehat{\mathbf{WQSym}}$, the linear endomorphisms that preserve some extra structure. Particularly important from this point of view are the coalgebra endomorphisms, whose classification is the object of the present section.

¿From now on, coalgebras C are coaugmented, counital and conilpotent. That is, writing Δ the coproduct and id_C the identity map of C: the coalgebra is equipped with a map η_C (the counit) from C to the ground field $\mathbf{Q}$ which satisfies

$$(\eta_C \otimes \mathrm{id}_C) \circ \Delta = \mathrm{id}_C = (\mathrm{id}_C \otimes \eta_C) \circ \Delta.$$

The ground field embeds (as a coalgebra) into C so that, canonically, $C = C^+ \oplus \mathbf{Q}$ with $C^+ := Ker\ \eta_C$ (coaugmentation) and, finally, writing $\overline{\Delta}$ the reduced coproduct ($\overline{\Delta}(x) := \Delta(x) - x \otimes 1 - 1 \otimes x$), for all $x \in C^+$, there exists an integer n (depending on x) such that $\overline{\Delta}^n(x) = 0$ (conilpotency). Coalgebra maps $\phi : C \to C'$ are required to preserve the coaugmentation and the counit, so that $\phi(C^+) \subset C'^+$.

Recall that $\mathrm{Sh}(A)$ is equipped with a coalgebra structure

$$\Delta(a_1 ... a_n) := \sum_{i=0}^{n} a_1 ... a_i \otimes a_{i+1} ... a_n \in \mathrm{Sh}(A) \otimes \mathrm{Sh}(A).$$

Its counit is the projection onto $\mathrm{Sh}_0(A) = \mathbf{Q}$ and we write

$$\mathrm{Sh}(A)^+ = \bigoplus_{n\geq 1} A^{\otimes n}.$$

The usual universal properties of the tensor algebra $T(A)$ as a free associative algebra over A (viewed as a vector space) dualize, and we have the adjunction property

$$\mathrm{Hom}_{\mathrm{lin}}(C^+, A) \cong \mathrm{Hom}_{\mathrm{coalg}}(C, \mathrm{Sh}(A)),$$

where C runs over coalgebras and $\mathrm{Hom}_{\mathrm{lin}}$, resp. $\mathrm{Hom}_{\mathrm{coalg}}$, stand for the set of linear maps, resp. coalgebra maps. In other terms, the coaugmentation coideal functor from coalgebras to vector spaces is left adjoint to the free coalgebra functor. Recall that in this statement coalgebra means coaugmented, counital and conilpotent coalgebra. The fact that we consider only conilpotent coalgebras is essential for the adjunction to hold, see e.g. [1] for details on the structure of cofree coalgebras in general. In particular, we get:

Corollary 4. *There is a canonical bijection*

$$\mathrm{Hom}_{\mathrm{lin}}(\mathrm{Sh}^+(A), A) \cong \mathrm{Hom}_{\mathrm{coalg}}(\mathrm{Sh}(A), \mathrm{Sh}(A)).$$

That is, a coalgebra endomorphism ϕ of $\mathrm{Sh}(A)$ is entirely determined by the knowledge of $f := \pi \circ \phi$, where we write π for the projection from $\mathrm{Sh}(A)$ to A orthogonally to $A^0 = \mathbf{Q}$ and to the $A^{\otimes n}$, $n > 1$. Conversely, any map $f \in \mathrm{Hom}_{\mathrm{lin}}(\mathrm{Sh}^+(A), A)$ determines a unique coalgebra endomorphism ϕ of $\mathrm{Sh}(A)$ by

$$\phi(a_1...a_n) := \sum_{i_1+...+i_k=n} f(a_1...a_{i_1}) \otimes \cdots \otimes f(a_{i_1+....+i_{k-1}+1}...a_n).$$

A triangularity argument that we omit shows that ϕ is a coalgebra automorphism if and only if the restriction of f to A is a linear isomorphism. For reasons that will become clear soon, we say that $f \in \mathrm{Hom}_{\mathrm{lin}}(\mathrm{Sh}^+(A), A)$ is tangent to identity if its restriction to A (that is to a linear endomorphism of A) is the identity map.

Recall that by natural endomophism of the functor Sh viewed as a functor from commutative nonunital algebras to coalgebras is meant a familly μ_A (indexed by commutative nonunital algebras A) of coalgebra endomorphisms of the $\mathrm{Sh}(A)$ commuting with the morphisms (from $\mathrm{Sh}(A)$ to $\mathrm{Sh}(B)$) induced by algebra maps (from A to B).

Theorem 5. *Let* **Coalg** *be the monoid of natural endomophisms of the functor* Sh *viewed as a functor from commutative nonunital algebras to coalgebras. Then, there is an isomorphism between* **Coalg** *and the monoid* **Diff** *of formal power series without constant term,* $\mathbf{Coalg} \cong X\mathbf{Q}[[X]]$ *equipped with the substitution product (for* $P(X), Q(X) \in X\mathbf{Q}[[X]]$, $P \circ Q(X) := P(Q(X))$.

In particular, the set $\mathbf{Coalg_1}$ *of tangent-to-identity natural endomorphisms of the functor* Sh *is a group canonically in bijection with the group* $\mathbf{Diff_1} = X + X^2\mathbf{Q}[[X]]$ *of tangent-to-identity formal diffeomorphisms.*

Let us prove first that $\mathbf{Coalg} \cong X\mathbf{Q}[[X]]$. Since we have a natural isomorphism $\mathrm{Hom}_{\mathrm{lin}}(\mathrm{Sh}^+(A), A) \cong \mathrm{Hom}_{\mathrm{coalg}}(\mathrm{Sh}(A), \mathrm{Sh}(A))$, **Coalg** is canonically in bijection with natural transformations from Sh^+ to the identity functor (viewed now as functors from commutative algebras to vector spaces). By Schur-Weyl duality, we get $\mathbf{Coalg} \cong \prod_{n\geq 1} \mathbf{WQSym}_{n,1}$. Identifying the unique surjection from $[n]$ to $[1]$ with the monomial X^n yields the bijection $\mathbf{Coalg} \cong X\mathbf{Q}[[X]]$.

We will write from now on ϕ_P for the element in $\mathrm{Hom}_{\mathrm{coalg}}(\mathrm{Sh}(A), \mathrm{Sh}(A))$ associated with a given formal power series $P(X) \in X\mathbf{Q}[[X]]$ and f_P for the corresponding element in $\mathrm{Hom}_{\mathrm{lin}}(\mathrm{Sh}^+(A), A)$.

Notice that for $P(X) = \sum_{i=1}^{\infty} p_i X^i$, the action of f_P and ϕ_P on an arbitrary tensor $a_1...a_n \in \mathrm{Sh}(A)$ can be described explicitely

$$f_P(a_1...a_n) = p_n \cdot (a_1 \cdot ... \cdot a_n) \in A, \tag{3}$$

$$\phi_P(a_1...a_n) = \sum_{k=1}^{n} \sum_{i_1+...+i_k=n} p_{i_1}...p_{i_k}(a_1 \cdot ... \cdot a_{i_1}) \otimes ... \otimes (a_{i_1+...+i_{k-1}+1} \cdot ... \cdot a_n) \tag{4}$$

This last formula describes the embedding of $\mathbf{Coalg}$ into $\widehat{\mathbf{WQSym}}$ induced by Schur-Weyl duality (the tensor product $(a_1 \cdot ... \cdot a_{i_1}) \otimes ... \otimes (a_{i_1+...+i_{k-1}+1} \cdot ... \cdot a_n)$ corresponding to the nondecreasing surjection from $[n]$ to $[k]$ sending the first i_1 integers to 1,..., the last i_k integers to k). This embedding is of course different from the one induced by the bijection with $\prod_{n\geq 1} \mathbf{WQSym}_{n,1}$ and corresponds to the fact that elements in $\mathbf{Coalg}$ can be represented equivalently by a f_P or a ϕ_P: the f_Ps are naturally encoded by elements in $\prod_{n\geq 1} \mathbf{WQSym}_{n,1}$ (Fla (3)), whereas the ϕ_Ps are most naturally encoded by elements in $\widehat{\mathbf{WQSym}}$ (Fla (4)).

Let us show now that, for arbitrary $P(X),\ Q(X) \in X\mathbf{Q}[[X]]$,

$$\phi_P \circ \phi_Q = \phi_{P(Q)}, \tag{5}$$

where $P(Q)(X) := P(Q(X))$. For an arbitrary commutative algebra A and $a_1, ..., a_n \in A$, we have indeed (with self-explaining notations for the coefficients of P and Q)

$$\pi \circ \phi_P \circ \phi_Q(a_1...a_n) =$$

$$= f_P(\sum_{k=1}^{n} \sum_{i_1+...+i_k=n} q_{i_1}...q_{i_k}(a_1 \cdot ... \cdot a_{i_1}) \otimes ... \otimes (a_{i_1+...+i_{k-1}+1} \cdot ... \cdot a_n))$$

$$= \sum_{k=1}^{n} \sum_{i_1+...+i_k=n} p_k q_{i_1}...q_{i_k}(a_1 \cdot ... \cdot a_n) = f_{P(Q)}(a_1...a_n) = \pi \circ \phi_{P(Q)}(a_1...a_n).$$

Thus, $\phi_P \circ \phi_Q = \phi_{P(Q)}$ and the theorem follows.

3. Formal diffeomorphisms and WQSym

We have shown that $\mathbf{Coalg}$ and $\mathbf{Diff}$ embed naturally into $\widehat{\mathbf{WQSym}}$ (Fla (4)). We have already noticed that they are actually embedded in $\widehat{\mathbf{IQSym}}$, where $\mathbf{IQSym}$ stands for the linear span of nondecreasing surjections. Since a nondecreasing surjection f from $[n]$ to $[k]$ is characterized by the number of elements $f_i := |f^{-1}(i)|$ in the inverse images of the elements of $i \in [k]$, nondecreasing surjections from $[n]$

to $[k]$ are in bijection with compositions of n of length k, that is, ordered sequences of integers $f_1, ..., f_k$ adding up to n. Said otherwise, nondecreasing surjections are naturally in bijection with a linear basis of **Sym** and **QSym**, respectively the Hopf algebra of noncommutative symmetric functions and the dual Hopf algebra of quasi-symmetric functions, see [7], although the linear embeddings of **Sym** and **QSym** into **WQSym** induced by the bijection between the basis and the embedding of **IQSym** into **WQSym** are not standard ones.

We shall return later on these various embeddings into **WQSym**; the present section studies the compatibility relations between the group structure of $\mathbf{Diff}_1$ and the coalgebra structure existing on **WQSym**.

Let us recall the relevant definitions. The word realization of **WQSym** to be introduced now will be useful when we will discuss later some of its combinatorial properties. We denote by $A = \{a_1 < a_2 < \dots\}$ an infinite linearly ordered alphabet and by A^* the corresponding set of words.

The *packed word* $u = \mathrm{pack}(w)$ associated with a word $w \in A^*$ is obtained by the following process. If $b_1 < b_2 < \cdots < b_r$ are the letters occuring in w, u is the image of w by the homomorphism $b_i \mapsto a_i$. For example, if $A = \mathbb{N}^*$, $pack(3\,5\,3\,8\,1) = 2\,3\,2\,4\,1$. A word u is said to be *packed* if $\mathrm{pack}(u) = u$. We denote by PW the set of packed words. With a word $u \in \mathrm{PW}$, we associate the noncommutative polynomial[2]

$$\mathbf{M}_u(A) := \sum_{\mathrm{pack}(w)=u} w\,. \tag{6}$$

For example, restricting A to the first five integers,

$$\begin{aligned} \mathbf{M}_{13132}(A) = \quad & 13132 + 14142 + 14143 + 24243 \\ & + 15152 + 15153 + 25253 + 15154 + 25254 + 35354. \end{aligned} \tag{7}$$

Packed words $u = u_1...u_n$ are in bijection with surjections: taking for A the set of integers, if $1, ..., p$ are the letters occuring in u, the surjection associated with u is simply the map from $[n]$ to $[p]$ defined by $f(i) := u_i$. The $\mathbf{M}_u$ can therefore be chosen as linear generators of **WQSym**. Since the product of two $\mathbf{M}_u$s is a linear combination of $\mathbf{M}_u$s, this presentation induces an algebra structure on **WQSym** and an algebra embedding into $\mathbf{Q}\langle A\rangle$. This algebra structure on **WQSym** is closely related to the Hopf algebra structure of $\mathrm{QSh}(A)$, see [14] for details. Since both presentations of **WQSym** ($\mathbf{M}_u$ or surjections) are equivalent, we will not distinguish between them, except notationally.

As for classical symmetric functions, the nature of the ordered alphabet A chosen to define word quasi-symmetric functions $\mathbf{M}_u(A)$ is largely irrelevant provided it has enough elements. We will therefore often omit the A-dependency and write simply $\mathbf{M}_u$ for $\mathbf{M}_u(A)$, except when we want to emphasize this dependency (and similarly for the other types of generalized symmetric functions we will have to deal with).

[2]As is customary in this theory, "polynomial" means a formal series of bounded degree in an infinite number of noncommuting variables, where each monomial of finite degree may carry a non zero scalar coefficient. We still denote by $Q\langle A\rangle$ the corresponding algebra. Since these are elements of a projective limit of polynomial rings, purists may want to call these objects *(noncommutative) prolynomials.*

The important point for us now is that **WQSym** carries naturally a Hopf algebra structure for the coproduct:

$$\Delta(\mathbf{M}_u) := \sum_{i=0}^{n} \mathbf{M}_{u_{|[1,i]}} \otimes \mathbf{M}_{\mathrm{pack}(u_{|[i+1,n]}))}. \tag{8}$$

Here, u is a packed word over the letters $1, ..., n$ and, for an arbitrary subset S of $[n]$, $u_{|S}$ stands for the word obtained from u by erasing all the letters that do not belong to S.

Lemma 6. *The direct sum of the spaces of nondecreasing surjections, and of the scalars,* **IQSym***, is a subcoalgebra of* **WQSym**. *It is a cofree coalgebra, cogenerated by the set $\Gamma \cong \mathbb{N}^+$ of "elementary" surjections γ_n from $[n]$ to $[1]$, $n \geq 1$. That is, as a coalgebra,* **IQSym** *identifies with $T(\Gamma)$ (the linear span of words over the alphabet of elementary surjections) equipped with the deconcatenation coproduct.*

In particular, **IQSym** is isomorphic as a coalgebra to **QSym**, the coalgebra of quasi-symmetric functions [8, 12, 21] and the embedding of **IQSym** in **WQSym** induces a coalgebra embedding of **QSym** in **WQSym**.

Recall that coalgebra means here coaugmented counital conilpotent coalgebra, so that the free coalgebra over a generating set X identifies with the tensor algebra over $\mathbf{Q}X$ equipped with the deconcatenation coproduct. The Lemma follows then from the definition of Δ. Indeed, if we write $\gamma_{i_1}...\gamma_{i_k}$ for the unique surjection f from $[i_1 + ... + i_k]$ to $[k]$ such that $f(1) = ... = f(i_1) := 1, \ \ldots, f(i_1 + ... + i_{j-1} + 1) = ... = f(i_1 + ... + i_k) := k$, then,

$$\Delta(\gamma_{i_1}...\gamma_{i_k}) = \sum_{j=0}^{k} \gamma_{i_1}...\gamma_{i_j} \otimes \gamma_{i_{j+1}}...\gamma_{i_k}.$$

Proposition 7. *The embedding of* $\mathbf{Diff}_1$ *into* $\widehat{\mathbf{IQSym}}$ *factorizes through the set of grouplike elements in* $\widehat{\mathbf{IQSym}}$ *(the same statement holds if we replace* **IQSym** *by the isomorphic coalgebra* **QSym***). In other terms, the group structure of* $\mathbf{Diff}_1$ *is compatible with the coalgebra structure of* **WQSym** *(resp.* **QSym***).*

Let $P(X) = X + \sum_{i>1} p_i X^i$ and $p_1 := 1$. Then, in the basis $\mathbf{M}_u$,

$$\phi_P = \sum_{n \geq 0} \sum_{k=1}^{n} \sum_{i_1+...+i_k=n} p_{i_1}...p_{i_k} M_{1^{i_1}...k^{i_k}},$$

where $1^{i_1}...k^{i_k}$ stands for the nondecreasing packed word with i_1 copies of 1, ..., i_k copies of k (so that e.g. $1^3 2^2 3^2 = 1112233$) with the convention that the component $n = 0$ of the sum contributes $1 \in \mathbf{Q}$ (this corresponds to $\phi_P(1) = 1$). We get

$$\Delta(\phi_P) = \sum_{n \geq 0} \sum_{k=1}^{n} \sum_{a+b=k} \sum_{i_1+...+i_k=n} p_{i_1}...p_{i_a} M_{1^{i_1}...a^{i_a}} \otimes p_{i_{a+1}}...p_{i_k} M_{1^{i_{a+1}}...(b-a)^{i_k}}$$
$$= \phi_P \otimes \phi_P.$$

Notice that, as a by-product, we have characterized the grouplike elements ϕ in $\widehat{\mathbf{WQSym}}$ which satisfy the compatibility property

$$\Delta(\phi) \circ \Delta(a_1...a_n) = \Delta \circ \phi(a_1...a_n). \tag{9}$$

In general, for ϕ in $\widehat{\mathbf{WQSym}}$ (not necessarily grouplike), equation (9) cannot hold if $\phi \notin \widehat{\mathbf{IQSym}}$ (this is because the deconcatenation coproduct Δ preserves the relative ordering of the a_is). The converse statement is true and follows from the definition of the coproduct on $\mathbf{WQSym}$ (its proof is left to the reader):

Lemma 8. *Equation* (9) *holds for all* $\phi \in \widehat{\mathbf{IQSym}}$*, This property characterizes* $\widehat{\mathbf{IQSym}}$ *as a subspace of* $\widehat{\mathbf{WQSym}}$.

Proposition 9. *The internal product (defined as the composition of surjections on* $\mathbf{IQSym}^+$*, the usual product on* $\mathbf{Q} = \mathbf{IQSym}_0 = \mathbf{IQSym} \cap \mathbf{WQSym}_0$ *–the product of elements in* $\mathbf{IQSym}^+$ *and* $\mathbf{Q}$ *is defined to be the null product) provides* $\mathbf{IQSym}$ *with a bialgebra*[3] *structure. That is, the coproduct* Δ *and the composition of surjections* $\circ$ *satisfy*

$$\Delta(f \circ g) = \Delta(f) \circ \Delta(g). \tag{10}$$

Indeed, by nonlinear Schur-Weyl duality, the identity is true if and only if the following identity holds for arbitrary A, and $a_1, ..., a_n$ in A

$$\Delta(f \circ g) \circ \Delta(a_1...a_n) = \Delta(f) \circ \Delta(g) \circ \Delta(a_1...a_n),$$

which follows from the previous Lemma and from the stability of $\mathbf{IQSym}$ by composition (the composition of two nondecreasing surjections is an nondecreasing surjection).

The identity map $I \in \widehat{\mathbf{IQSym}}$ (the sum of all identity maps on the finite sets $[n]$) is a unit for $\circ$ and behaves as a grouplike element for Δ. However, $I \notin \mathbf{IQSym}$ and problems arise if one tries to provide $\mathbf{IQSym}$ with a classical *graded* unital bialgebra structure. A natural gradation of $\mathbf{IQSym}$ would be the relative degree of surjections (since the relative degree of the composition of two surjections f and g is the sum of their relative degrees). However, for this gradation, each graded component of $\mathbf{IQSym}$ is infinite dimensional (even in degree 0), so that many of the usual arguments regarding graded Hopf algebras do not apply directly to $\mathbf{IQSym}$.

Since we aim at providing a group-theoretical picture of the theory of shuffle algebras, our final goal is to understand the fine structure of the image of $\mathbf{Diff}$ in $\widehat{\mathbf{IQSym}}$. The next section aims at clarifying these questions.

[3] By "bialgebra", we simply mean in the present article a compatible product and coproduct as in identity (10), without requiring extra properties (very often one requires the coproduct and the product to have also compatibility properties with the unit of the algebra and the counit of the coalgebra).

4. Natural coderivations and the Faà di Bruno algebra

In the previous section, we have characterized the natural coalgebra endomorphisms of shuffle algebras, or, equivalently, grouplike elements in $\widehat{\mathbf{IQSym}}$. We have also shown that the tangent-to-identity elements form a group isomorphic to the group of tangent-to-identity formal diffeomorphisms. We are going to study now the corresponding Lie algebra L of natural coderivations of shuffle algebras.

Recall the canonical isomorphism $\mathbf{IQSym} \cong T(\mathbf{Q}\Gamma)$ (with $\Gamma \cong \mathbb{N}^*$). Let $S(\Gamma)$ stand for the subspace of symmetric tensors in $T(\mathbf{Q}\Gamma)$ and **SIQSym** be the corresponding subspace of **IQSym**. By construction, the embedding of **Diff** into **IQSym** factorizes through **SIQSym** (see Eq. (4)). Since symmetric tensors form a subcoalgebra of the tensor algebra for the deconcatenation coproduct and since the composition of two elements in **SIQSym** is still in **SIQSym**, the following Lemma is a consequence of our previous results.

Lemma 10. *The embedding of* **SIQSym** *into* **IQSym** *is an embedding of bialgebras (for the composition product).*

Let us call tangent-to-identity an element μ in $\widehat{S(\Gamma)}$ if $\mu - I$ is a (possibly infinite) linear combination of nondecreasing strict surjections (nondecreasing surjections from $[n]$ to $[m]$ with $n > m$).

A coderivation D in $\mathrm{Sh}(A)$ (that is, a linear endomorphism such that $\Delta \circ D = (D \otimes I + I \otimes D) \circ \Delta$, where I stands for the identity map) is called infinitesimal if its restriction to $A \subset \mathrm{Sh}(A)$ is the null map. As usual, a natural coderivation of the shuffle algebras is a familly of coderivations (of the $\mathrm{Sh}(A)$) commuting with the morphisms induced by algebra maps (from A to B, where A and B run over commutative nonunital algebras).

Lemma 11. *Natural tangent-to-identity coalgebra endomorphisms of shuffle algebras identify with tangent-to-identity grouplike elements in* $\widehat{\mathbf{SIQSym}} \cong \widehat{S(\Gamma)}$. *The corresponding Lie algebra of primitive elements in* $\widehat{S(\Gamma)}$ *is the Lie algebra of natural infinitesimal coalgebra coderivations of the shuffle algebras. It is canonically in bijection with the Lie algebra of formal power series* $X^2\mathbf{Q}[[X]]$ *equipped with the Lie bracket* $[X^m, X^n] := (m-n)X^{m+n-1}$.

The Lemma follows from the general property according to which, in a bialgebra, grouplike elements and primitive elements are in bijection through the logarithm and exponential maps, provided these maps make sense (that is, provided no convergence issue of the series arises). This is because, formally, for ϕ a grouplike element,

$$\Delta(\log(\phi)) = \log(\Delta(\phi)) = \log(\phi \otimes \phi) = \log(\phi) \otimes I + I \otimes \log(\phi),$$

since $\log(ab) = \log(a) + \log(b)$ when a and b commute and since I is the unit element for the composition product.

The formal convergence of the series under consideration in the present case is ensured by the fact that a surjection from n to $p < n$ can be written as the product of at most $n - p$ strict surjections (so that the coefficient of such a surjection in the expansion of $\log(\phi)$ is necessarily finite and equal to its coefficient in the expansion of the truncation of the logarithmic series at order $n-p$).

The last statement of the Lemma follows from the isomorphism between tangent-to-identity coalgebra endomorphisms of shuffle algebras and tangent-to-identity formal diffeomorphisms. It can also be deduced directly from the adjunction property (dual to the one according to which derivations in the tensor algebra are in bijection with linear morphisms from V to $T(V)$): writing $\mathrm{Coder}^+(\mathrm{Sh}(A))$ for the coderivations of $\mathrm{Sh}(A)$ vanishing on $\mathbf{Q}$, we have $\mathrm{Coder}^+(\mathrm{Sh}(A)) \cong \mathrm{Lin}(\mathrm{Sh}^+(A), A)$, which implies, by nonlinear Schur-Weyl duality that natural coalgebra coderivations of the shuffle algebras are canonically in bijection with $X\mathbf{Q}[[X]]$.

This bijection with $X\mathbf{Q}[[X]]$ can be made explicit: dualizing the formula for the derivation associated with a map $f : V \longrightarrow T(V)$

$$f(v_1...v_n) := \sum_{i=1}^{n} v_1...v_{i-1}f(v_i)v_{i+1}...v_n,$$

we get, for $P = \sum_{i\geq 1} p_i X^i$

$$D_P(a_1...a_n) = \sum_{i=1}^{n} \sum_{j=1}^{n-i+1} p_i a_1...a_{j-1}(a_j \cdot ... \cdot a_{j+i-1})a_{j+i}...a_n.$$

In particular, the restriction of ϕ_P and D_P to maps from $\mathrm{Sh}(A)$ to A agree and are both given by

$$\phi_P(a_1...a_n) = D_P(a_1...a_n) = p_n a_1 \cdot ... \cdot a_n.$$

The simplest example of a coderivation is for $P(X) = X$: it is the degree operator, $Y := D_X$,

$$Y(a_1...a_n) = \sum_{i=1}^{n} a_1...a_{i-1}I(a_i)a_{i+1}...a_n = n\ a_1...a_n.$$

Similarly, $D_{\lambda X}(a_1...a_n) = n \cdot \lambda\ (a_1...a_n)$. In general we have, for arbitrary polynomials P, Q and $\lambda \in \mathbf{Q}$,

$$D_P + \lambda D_Q = D_{P+\lambda Q}.$$

The description of the Lie algebra structure on $X\mathbf{Q}[[X]]$ induced by the isomorphism with the Lie algebra of natural coalgebra coderivations follows from the explicit formula for the action of coderivations ($[D_{X^m}, D_{X^n}] = (m-n)D_{X^{m+n-1}}$) but can also be deduced from the fact that composition of coalgebra endomorphisms is reflected in the composition of formal power series. Recall indeed that the set of formal power series $X + X^2\mathbf{Q}[[X]]$ equipped with the composition product is the group of characters of the Faà di Bruno Hopf algebra, see e.g. [5].

Summarizing our previous results, we get:

Theorem 12. *The Lie algebra of natural infinitesimal coalgebra coderivations of shuffle algebras is naturally isomorphic to (the completion of) the Lie algebra generated by the X^n, $n > 1$, with Lie bracket $[X^m, X^n] := (m-n)X^{m+n-1}$. Equivalently, it is isomorphic to (the completion of) the Lie algebra of primitive elements in the Hopf algebra dual to the Faà di Bruno Hopf algebra.*

Here, "completion" is understood with respect to the underlying implicit grading of these Lie algebras and Hopf algebras (e.g. X^n is naturally of degree $n-1$, see [5] for details).

5. Deformations of shuffles

Let us restrict again our attention to tangent-to-identity coalgebra automorphisms of the $\mathrm{Sh}(A)$. Any such Φ_P (with $P(X)-X\in X^2\mathbf{Q}[[X]]$) defines a natural deformation of Sh, that is, a new functor from commutative algebras to Hopf algebras

$$\mathrm{Sh}_P(A)=(\mathrm{Sh}(A),\Delta,\sqcup\!\sqcup_P),$$

that is, $\mathrm{Sh}_P(A)$ identifies with $\mathrm{Sh}(A)$ (and with $T(A)$ equipped with the deconcatenation coproduct) as a coalgebra, but carries a new product defined by conjugacy

$$x\sqcup\!\sqcup_P y:=\phi_P(\phi_P^{-1}(x)\sqcup\!\sqcup\phi_P^{-1}(y)).$$

For the sake of completeness, let us check explicitely the compatibity relation of the product $\sqcup\!\sqcup_P$ and the coproduct: since ϕ_P^{-1} is a coalgebra automorphism,

$$\begin{aligned}\Delta(x\sqcup\!\sqcup_P y)=\Delta\circ\phi_P(\phi_P^{-1}(x)\sqcup\!\sqcup\phi_P^{-1}(y))&=(\phi_P\otimes\phi_P)\circ\Delta(\phi_P^{-1}(x)\sqcup\!\sqcup\phi_P^{-1}(y))\\&=(\phi_P\otimes\phi_P)\circ(\Delta(\phi_P^{-1}(x))\sqcup\!\sqcup\Delta(\phi_P^{-1}(y)))\\&=(\phi_P\otimes\phi_P)\circ((\phi_P^{-1}\otimes\phi_P^{-1})\circ\Delta(x)\sqcup\!\sqcup(\phi_P^{-1}\otimes\phi_P^{-1})\circ\Delta(y))\\&=\Delta(x)\sqcup\!\sqcup_P\Delta(y).\end{aligned}$$

Definition 13. *The Hopf algebra* $\mathrm{Sh}_P(A)$ *is called the P-twisted shuffle algebra. It is isomorphic to* $\mathrm{Sh}(A)$ *as a Hopf algebra.*

It inherits therefore all the properties of $\mathrm{Sh}(A)$. The reader is referred to Reutenauer's book [19] for a systematic study of shuffle algebras. As an algebra, $\mathrm{Sh}(A)$ is, for example, a free commutative algebra over a set of generators parametrized by Lyndon words.

The fundamental example of a deformation is provided by the "q-exponential" map

$$E_q:=\sum_{n\in\mathbb{N}^*}\frac{q^{n-1}x^n}{n!}$$

which interpolates between the identity $E_0=x$ and $E_1=e^x-1$. The corresponding isomorphism between $\mathrm{Sh}(A)$ and $\mathrm{Sh}_{E_q}(A)$ is then given by

$$\phi_{E_q}(a_1...a_n)=\sum_{\mathcal{P}}\frac{q^{n-k}}{P_1!...P_k!}a_{P_1}...a_{P_k},$$

where $\mathcal{P}=(P_1,...,P_k)$ runs over the nondecreasing partitions of $[n]$ ($P_1\coprod...\coprod P_k=[n]$ and $P_i<P_j$ if $i<j$; $a_{P_i}:=\prod\limits_{j\in P_i}a_j$ and $P_1!$ is a shortcut for $|P_1|!$.

Lemma 14. *When $q=1$,* $\mathrm{Sh}_{E_1}(A)$ *identifies with* $\mathrm{QSh}(A)$, *the quasi-shuffle algebra over A, whose product, written* $\uplus$, *is defined recursively by*

$$a_1...a_n\uplus b_1...b_m:=$$
$$a_1(a_2...a_n\uplus b_1...b_m)+b_1(a_1...a_n\uplus b_2...b_m)+(a_1\cdot b_1)(a_2...a_n\uplus b_2...b_m).$$

The exponential map ϕ_{E_1} generalizes the Hoffman isomorphism between Sh(A) and QSh(A) introduced and studied in [11] in the case where A is a locally finite dimensional graded connected algebra. Using a graded connected commutative algebra A (instead of an arbitrary commutative algebra as in the present article), although a strong restriction in view of applications, has some technical advantages: it allows, for example, to treat directly QSh(A) as a graded connected Hopf algebra, making possible the use of structure theorems for such algebras (Cartier-Milnor-Moore, Leray...). The classical illustration of these phenomena is provided by the algebra of quasi-symmetric functions (the quasi-shuffle algebra over the monoid algebra of the positive integers) and the dual algebra of noncommutative symmetric functions: using the gradation on **QSym** induced by the one of the integers, $\mathbb{N}^*$, the exponential/logarithm transform amounts then to a mere change of basis (between a family of grouplike vs primitive generators) see [8, 7, 11] for details.

The proof amounts to showing that

$$\phi_{E_1}(a_1...a_n \sqcup\!\sqcup a_{n+1}...a_{n+m}) = \phi_{E_1}(a_1...a_n) \uplus \phi_{E_1}(a_{n+1}...a_{n+m}).$$

Let us write $R_1...R_k$ for an arbitrary partition of $[n+m]$ such that for $1 \leq i < j \leq n$ or $n+1 \leq i < j \leq n+m$ $i \in R_p,\ j \in R_q \Rightarrow p \leq q$. The problem amounts to computing the coefficient of $a_{R_1}...a_{R_k}$ in the expansion of the left and right-hand sides of the equation. We leave to the reader the verification that only such tensors appear in these expansions. The coefficient is in both cases $\frac{1}{P_1!...P_k!}\frac{1}{Q_1!...Q_k!}$, where $P_i := R_i \cap [n]$, $Q_i := R_i \cap \{n+1, ..., n+m\}$. This is straightforward for the right-hand side (the reader not familiar with quasi-shuffle products is encouraged to write down the tedious but straightforward details of the proof -using e.g. the recursive definition of $\uplus$). For the left-hand side, it follows from the identity $\binom{|R_i|}{|P_i|} \times \frac{1}{R_i!} = \frac{1}{P_i!Q_i!}$ and the fact that the number of words in the expansion of a shuffle product $x_1...x_l \sqcup\!\sqcup y_1...y_k$ is $\binom{l+k}{k}$.

As we shall see in the sequel, even in the well-known special case of a graded algebra, the point of view developed in the present article is not without interest: being more general and conceptual than usual approaches to quasi-shuffle algebras, it allows the derivation of new insights on the fine structure of their operations, refining the results already obtained in [14].

Interesting new phenomena do actually occur as soon as one considers natural linear endomorphisms of shuffle algebras. We have already recalled from [14] that, by Schur-Weyl duality, they belong to **WQSym**, which inherits an associative (convolution) product from the Hopf algebra structure of the Sh(A): for $f \in \mathbf{WQSym}_n$, $g \in \mathbf{WQSym}_m$ and arbitrary $a_1, ..., a_{n+m} \in A$, where A is an arbitrary commutative algebra,

$$f \sqcup\!\sqcup g(a_1...a_{n+m}) := f(a_1...a_n) \sqcup\!\sqcup g(a_{n+1}...a_{n+m}).$$

When f and g belong to **FQSym**, the subset of permutations in **WQSym**, this convolution product has a simple expression and defines the "usual" product on **FQSym**, see e.g. [12, 2]. Writing $\mathrm{Sh}_{n,m}$ for the set of (n, m)-shuffles (that is the elements σ in the symmetric group S_{n+m} of order $n + m$ such that $\sigma(1) < ... < \sigma(n)$

and $\sigma(n+1) < ... < \sigma(n+m)$), we get

$$f \sqcup\!\sqcup g = \sum_{\zeta \in \mathrm{Sh}_{n,m}} \zeta \circ (f \cdot g),$$

where $f \cdot g$ stands for the "concatenation" of permutations: $f \cdot g(i) := f(i)$ for $i \leq n$ and $f \cdot g(i) := n + g(i-n)$ else.

Recall that word and free quasisymmetric functions (**WQSym** and **FQSym**) carry a coproduct, defined on packed words f over k letters by

$$\Delta(f) := \sum_{i=0}^{k} f_{|\{1,\dots,i\}} \otimes \mathrm{pack}(f_{|\{i+1,\dots,k\}}),$$

this coproduct together with $\sqcup\!\sqcup$ defines a graded Hopf algebra structure on both **WQSym** and **FQSym** (the grading is then defined by requiring a surjection from $[n]$ to $[p]$ to be of degree n). In particular, the embedding $\mathbf{FQSym} \subset \mathbf{WQSym}$ is an embedding of Hopf algebras for these structures. Recall however that $\sqcup\!\sqcup$ *is not* the usual product used when studying **WQSym**, see below for details.

The following lemma is instrumental and will prove quite useful. Its proof is left to the reader.

Lemma 15. *For f a nondecreasing surjection ($f \in \mathbf{IQSym}$) and $g \in \mathbf{WQSym}$,*

$$\Delta(f \circ g) = \Delta(f) \circ \Delta(g).$$

Notice that the Lemma would not hold with f arbitrary in **WQSym**.

¿From our previous considerations, *any* formal power series in $X\mathbf{Q}[[X]]$ will allow us to define a new convolution product on **WQSym** associated with the P-twisted Hopf algebra structure of the $\mathrm{Sh}_P(A)$. This new product, written $\sqcup\!\sqcup_P$ (resp. $\uplus$ when $P = E_1$, resp. $\sqcup\!\sqcup_q$ when $P = E_q$) is defined by

$$\forall f \in WQSym_n,\ g \in WQSym_m,$$

$$f \sqcup\!\sqcup_P g(a_1 ... a_{m+n}) := f(a_1 ... a_n) \sqcup\!\sqcup_P g(a_{n+1} ... a_{n+m}),$$

(the product $f \sqcup\!\sqcup_P g$ acts as the null map on tensors of length different from $n+m$).

The following result, although elementary, is stated as a theorem in view of its importance:

Theorem 16. *For an arbitrary $P \in X + X^2\mathbf{Q}[[X]]$, the composition map*

$$f \longmapsto \Phi_P(f) = f_P := \phi_P \circ f$$

induces an isomorphism of bialgebras from $(\mathbf{WQSym}, \Delta, \sqcup\!\sqcup)$ to $(\mathbf{WQSym}, \Delta, \sqcup\!\sqcup_P)$. For $P = E_1$ (resp. $P = E_q$) , we will write simply $\Phi_1(f)$ (resp. $\Phi_p(f)$) for $\Phi_P(f)$. This isomorphism is equivariant with respect to the composition product:

$$\phi_P(f \circ g) = \phi_P(f) \circ g.$$

The compatibility with the coproduct follows from Lemma 15, from the definition of f_P as the composition of f with a sum of nondecreasing surjections, and from the fact that $\Delta(\phi_P) = \phi_P \otimes \phi_P$. On an other hand, the definition of the twisted product $\sqcup\!\sqcup_P$ implies

$$f_P \sqcup\!\sqcup_P g_P = \phi_P \circ (f \sqcup\!\sqcup g) = (f \sqcup\!\sqcup g)_P.$$

The following corollaries are motivated by the key role of **FQSym** and **WQSym** in the theory of noncommutative symmetric functions and their various application fields:

Corollary 17. *Any $P \in X + X^2\mathbf{Q}[[X]]$ induces a Hopf algebra embedding of $(\mathbf{FQSym}, \Delta, \sqcup\!\sqcup)$ into $(\mathbf{WQSym}, \Delta, \sqcup\!\sqcup_P)$. This embedding is S_n-equivariant: for $\sigma, \beta \in S_n = \mathbf{FQSym}_n$, we have:*

$$(\sigma \circ \beta)_P = \sigma_P \circ \beta.$$

Corollary 18. *For $P = E_1$, we get that $(\mathbf{FQSym}, \Delta, \sqcup\!\sqcup)$ embeds naturally into $(\mathbf{WQSym}, \Delta, \uplus)$. As in the previous corollary, this embedding is S_n-equivariant.*

These corollaries allow to give an explicit formula for the embeddings. Indeed, for an arbitrary $\sigma \in S_n$, we get (writing 1_n the identity permutation in S_n)

$$\sigma_P = (1_n)_P \circ \sigma.$$

Since $(1_n)_P$ is simply the component of ϕ_P in $\mathbf{WQSym}_n$, we get finally

$$\sigma_P = \sum_{k=1}^{n} \sum_{i_1+\ldots+i_k=n} p_{i_1} \ldots p_{i_k} 1^{i_1} \ldots k^{i_k} \circ \sigma,$$

where we write $1^{i_1} \ldots k^{i_k}$ for the surjection sending the first i_1 integers to 1, ..., the integers from $i_1 + \ldots + i_{k-1} + 1$ to n to k. For E_q this formula simplifies:

Lemma 19. *Let $\sigma \in S_n$ and $\tau \in \mathbf{WQSym}_n$. We shall say that $\tau \propto \sigma$ if for all $1 \leq i, j \leq n$, $\sigma(i) < \sigma(j) \Rightarrow \tau(i) \leq \tau(j)$. We also set $\tau! := \prod_{i=1}^{max(\tau)} |\tau^{-1}(\{i\})|!$ and $r(\tau)$ for the relative degree of τ. Then, the Hopf algebra embedding Φ_p from **FQSym** into **WQSym** is given by*

$$\Phi_p(\sigma) = \sum_{\tau \propto \sigma} \frac{q^{r(\tau)}\tau}{\tau!}.$$

Other consequences of the existence of such embeddings will be drawn in the sequel.

6. Structure of twisted shuffle algebras

The map ϕ_P defines an isomorphism from $\mathrm{Sh}(A)$ to $\mathrm{Sh}_P(A)$ for an arbitrary commutative algebra A and an isomorphism between **WQSym** equipped with the shuffle product $\sqcup\!\sqcup$ to **WQSym** equipped with the twisted shuffle product $\sqcup\!\sqcup_P$.

In this section, we briefly develop the consequences of these isomorphisms and recover, among others, the results of [14] on projections onto the indecomposables in $\mathrm{QSh}(A)$.

Recall from [17, 18] that $e_1 := \log^{\sqcup\!\sqcup}(Id)$ (the logarithm of the identity map of $\mathrm{Sh}(A)$ computed using the shuffle product $\sqcup\!\sqcup$) is a canonical section of the projection from $\mathrm{Sh}(A)$ to the indecomposables $\mathrm{Sh}(A)^+/(\mathrm{Sh}(A)^+)^2$. In particular, due to the structure theorems for graded connected Hopf algebras over a field of characteristic 0 (Leray, in that particular case), $\mathrm{Sh}(A)$ is a free commutative algebra over the image of e_1. Equivalently, e_1 is the projection on the eigenspace of eigenvalue k of the k-th Adams operation, that is, the k-th power of the identity $(Id)^{\sqcup\!\sqcup k}$.

These properties are clearly invariant by conjugacy and we get, since $\phi_P \circ Id \circ \phi_P^{-1} = Id$, the following description of $\mathrm{Sh}_P(A)$ as a free commutative algebra:

Proposition 20. *For an arbitrary tangent-to-identity P, $e_1 := \log^{\sqcup\!\sqcup_P}(Id)$ (the logarithm of the identity for the $\sqcup\!\sqcup_P$ product) is a section of the projection from $\mathrm{Sh}_P(A)$ to the indecomposables $\mathrm{Sh}_P(A)^+/(\mathrm{Sh}_P(A)^+)^2$. In particular, $\mathrm{Sh}_P(A)$ is a free commutative algebra over the image of e_1. Equivalently, e_1 is the projection on the eigenspace associated with the eigenvalue k of the k-th Adams operation, that is, the k-th power of the identity $(Id)^{\sqcup\!\sqcup_P k}$.*

The particular case of the quasi-shuffle algebra was investigated in [14]. The projection e_1 can then be computed explicitly. Recall that a surjection f from $[n]$ to $[p]$ has a descent in position i if and only if $f(i) > f(i+1)$. Let us call conjugate projection and write $\tilde{f}$ for the projection from $[n]$ to $[p]$ defined by: $\tilde{f}(i) := f(n-i)$. We have:

Proposition 21. *In* **WQSym** *equipped with the quasi-shuffle $\uplus$,*

$$e_1 := \log^{\uplus}(Id) = \sum_{n\geq 1} \frac{1}{n} \sum_{I \models n} \frac{(-1)^{l(I)-1}}{\binom{n-1}{l(I)-1}} \sum_{\mathrm{Des}(f)=[n]-\{i_{l(I)},\dots,i_{l(I)}+\dots+i_1\}} \tilde{f},$$

where $I \models n$ means that $I = (i_1, \dots, i_{l(I)})$ is a composition of n.

To start investigating the word interpretation of **WQSym** and the combinatorial meaning of the formulas and results obtained so far, recall that, as any formula regarding **WQSym**, this proposition can be translated into a result on words (and actually also into a result on Rota–Baxter algebras, due to the relationship established in [3] between **WQSym** and free Rota–Baxter algebras).

Recall that the elements of **WQSym** can be realized as formal sums of words over a totally ordered alphabet X. For example, the identity map $\mathrm{Id} \in \widehat{\mathbf{WQSym}}$ identifies under this correspondence with the formal sum of all nondecreasing words over X.

When the alphabet is taken to be the sequence of values of a function from $[n-1]$ into an associative algebra, this formal sum identifies with the n-th value of the function (unique, formal) solution to the recursion $F = 1 + S(F \cdot f)$, where S is the summation operator $S(f)(j) := \sum_{i=1}^{j-1} f(i)$, $S(f)(1) := 0$. That is,

$$F(k) = 1 + \sum_{i=1}^{k-1} \sum_{1\leq a_1 < \dots < a_k \leq k-1} f(a_1)\dots f(a_k).$$

Since the concatenation product of words induces an associative product on **WQSym** that identifies with $\uplus$ [2], we get finally that e_1 computes in that case $\log(F)(n)$. This phenomenon was studied recently in detail in [4], to which we refer for details.

7. Gradations

In the context of shuffle algebras, the conjugacy map by ϕ_P, for an arbitrary tangent-to-identity P, maps the degree operator Y on $\mathrm{Sh}(A)$ to a degree operator $Y_P := \phi_P \circ Y \circ \phi_P^{-1}$ on $\mathrm{Sh}_P(A)$. That is, more explicitly:

Proposition 22. *The operator $Y_P := \phi_P \circ Y \circ \phi_P^{-1}$ acting on $\mathrm{Sh}_P(A)$ is a derivation and a coderivation which leaves invariant the subspaces $\mathrm{Sh}_P^{\leq n}(A) := \bigoplus_{i\leq n} A^{\otimes n}$. Its action is diagonalizable, with eigenvalues $i \in \mathbb{N}$. The eigenspaces for the eigenvalues 0 and 1 are the scalars, resp. A. In general, the eigenspace for the eigenvalue n is contained in $\mathrm{Sh}_P^{\leq n}(A)$ and its intersection with $\mathrm{Sh}_P^{\leq n-1}(A)$ is the null vector space, more precisely:*

$$\mathrm{Sh}_P^{\leq n}(A) = \mathrm{Sh}_P^{\leq n-1}(A) \oplus Ker(Y_p - nId).$$

Concretely, conjugacy by ϕ_P defines an isomorphism between $A^{\otimes n} \subset \mathrm{Sh}(A)$ and the eigenspace associated with the eigenvalue n of Y_P in $\mathrm{Sh}_P(A)$. The conjugacy map can be described explicitely as follows:

Proposition 23. *For $U \in X + X^2\mathbf{Q}[[X]]$ (or more generally in $\mathbf{Q}^*X + X^2\mathbf{Q}[[X]]$) and V an arbitrary formal power series without constant term,*

$$\phi_U^{-1} \circ D_V \circ \phi_U = D_{\frac{V\circ U}{U'}}.$$

By linearity of D and (formal) continuity of the action by conjugacy, it is enough to prove the formula when $V = X^p$. We denote by W the inverse of U for the composition and write u_i the coefficients of U, and similarly for V and W. Then,

$$\pi \circ \phi_W \circ D_{X^p} \circ \phi_U(a_1...a_n)$$
$$= f_W \circ D_{X^p}(\sum_{k=1}^{n} \sum_{i_1+...+i_k=n} u_{i_1}...u_{i_k}(a_1 \cdot ... \cdot a_{i_1})...(a_{i_1+...+i_{k-1}+1} \cdot ... \cdot a_n))$$
$$= \sum_{k=p}^{n} \sum_{i_1+...+i_k=n} (k-p+1)w_{k-p+1}u_{i_1}...u_{i_k}(a_1 \cdot ... \cdot a_n),$$

so that $\pi \circ \phi_W \circ D_{X^p} \circ \phi_U$ is the linear map associated to the formal power series:

$$\sum_{k=p}^{\infty}(k-p+1)w_{k-p+1}U^k = \big(\sum_{k=p}^{\infty}(k-p+1)w_{k-p+1}X^k\big) \circ U$$
$$= \big(\sum_{i=1}^{\infty} iw_iX^{i-1+p}\big) \circ U = (X^pW') \circ U = U^p \cdot (W' \circ U) = \frac{U^p}{U'}.$$

Hence,

$$\phi_U^{-1} \circ D_{X^p} \circ \phi_U = D_{\frac{U^p}{U'}},$$

and the proposition follows.

In particular, taking $P = E_1$, we get:

Proposition 24. *The eigenspaces of the coderivation $D_{(1+X)\ln(1+X)}$ provide the quasi-shuffle algebras* $\mathrm{QSh}(A)$ *with a grading and, more precisely, provide the triple* $(\mathrm{QSh}(A), ⧢, \Delta)$ *with the structure of graded connected commutative Hopf algebra.*

Indeed, with $D = \psi \circ D_X \circ \psi^{-1} = \psi \circ Y \circ \psi^{-1}$ and $\psi := \phi_{\exp(X)-1}$,

$$D = \phi^{-1}_{\ln(1+X)} \circ D_X \circ \phi_{\ln(1+X)} = D_{(1+X)\ln(1+X)}.$$

Notice that, since $(1+X)\ln(1+X) = 1 + \sum_{k+2}^{\infty} \frac{(-1)^k}{k(k+1)} X^k$,

$$D_{(1+X)\ln(1+X)}(a_1 \ldots a_n) = n \cdot a_1 \ldots a_n + \sum_{i=2}^{n} \sum_{j=1}^{n-i+1} \frac{(-1)^i}{i(i-1)} a_1 \ldots a_{j-1}(a_j \cdot \ldots \cdot a_{j+i-1}) a_{j+i} \ldots a_n.$$

8. A new realization of **Sym**

In the last sections, we develop some combinatorial applications of our previous results. We will focus mainly on the consequences of Lemma 19, that is, the existence of a new isomorphic embedding of **FQSym** into **WQSym**.

The present section explains briefly how these results translate in terms of *polynomial realizations* of these algebras. In particular, we emphasize that the previous embedding gives rise to *new* realizations of **Sym** and **FQSym** that will appear in the forthcoming section to be meaningful for the combinatorial study of the Hausdorff series.

Recall that **Sym**, the Hopf algebra of noncommutative symmetric functions, is the free associative algebra generated by a sequence S_i, $i \in \mathbb{N}^*$ of divided powers ($\Delta(S_n) := \sum_{i=0}^{n} S_i \otimes S_{n-i}$, where $S_0 := 1 \in \mathbf{Q}$). In [7], it has been shown that this Hopf algebra could bring considerable simplifications in the analysis of the so-called continuous BCH (Baker-Campbell-Hausdorff) series, the formal series $\Omega(t) = \log X(t)$ expressing the logarithm of the solution of the (noncommutative) differential equation $X'(t) = X(t)A(t)$ $(X(0) = 1)$ as iterated integrals of products of factors $A(t_i)$. The new polynomial realization of **Sym** to be introduced will lead instead to a straightforward proof of Goldberg's formula for the coefficients of the (usual) Hausdorff series.

This algebra **Sym** can be embedded as a Hopf subalgebra into **FQSym** by sending S_n to the identity element in the symmetric group of order n. This results into the usual polynomial realization of **Sym** introduced in [7] (that is, its realization through an embedding into the algebra of noncommutative polynomials $\mathbf{Q}\langle X \rangle$) sending S_n to the sum of all nondecreasing words of length n. We refer e.g. to [15] for details.

Instead of doing so, we may now take advantage of Lemma 19 and define a new polynomial realization of **Sym** using the existence of an isomorphic embedding Φ_1 of **FQSym** into **WQSym**:

$$\hat{S}_n = \sum_{u \text{ nondecreasing},\ |u|=n} \frac{1}{u!} \mathbf{M}_u, \tag{11}$$

where for notational convenience we write $\hat{S_n}$ for $\Phi_1(S_n)$ (and similarly for the images by Φ_1 of the other elements of **Sym** and **FQSym** in **WQSym**). In view of Fla (6), we have equivalently

$$\hat{\sigma}_t := \sum_{n\geq 0} t^n \hat{S}_n = e^{tx_1}e^{tx_2}\cdots = \prod_{i\geq 1}^{\rightarrow} e^{tx_i}\,. \tag{12}$$

Notice that $\hat{\sigma}_t$ is (as expected) a grouplike element for the standard coproduct of noncommutative polynomials for which letters x_i are primitive.

An interesting feature of this realization is that $\Phi := \log\hat{\sigma}_1$ is now the Hausdorff series

$$\Phi = \log(e^{x_1}e^{x_2}\cdots) = H(x_1, x_2, x_3, \dots)\,. \tag{13}$$

Moreover, two nondecreasing words v and w such that $\mathrm{pack}(v) = \mathrm{pack}(w) = u$ have the same coefficient in $\hat{\sigma}_1$, that is,

$$\frac{1}{u!}, \quad \text{where } u! := \prod_i m_i(u)! \tag{14}$$

and $m_i(u)$ is the number of occurences of i in u.

The Hausdorff series can now be expanded in the basis $\mathbf{M}_u$ of **WQSym** as

$$\Phi = \sum_u c_u \mathbf{M}_u \tag{15}$$

and one may ask whether the previous formalism can shed any light on the coeffients c_u. There is actually a formula for c_u, due to Goldberg [9], and reproduced in Reutenauer's book [19, Th. 3.11 p. 63]. This formula, which was obtained as a combinatorial *tour de force*, will be shown in the sequel to be a direct consequence of our previous results.

9. Goldberg's formula revisited

Let us fix first some notations. For $I = (i_1, ..., i_r)$, we set $S^I := S_{i_1}...S_{i_r}$; we also write $\ell(I) = r$ and $|I| = i_1 + ... + i_r$ (so that $I \vDash |I|$). By definition,

$$\Phi = \log(1 + \hat{S}_1 + \hat{S}_2 + \cdots) = \sum_{r\geq 1} \frac{(-1)^{r-1}}{r} \sum_{\ell(I)=r} \hat{S}^I = \int_{-1}^{0} \left(\sum_I t^{\ell(I)}\hat{S}^I\right)\frac{dt}{t} \tag{16}$$

so that the coefficient c_u of $\mathbf{M}_u$ in the Hausdorff series is, denoting by $\mathbf{N}_u$ the dual basis of $\mathbf{M}_u$,

$$c_u = \int_{-1}^{0} \left\langle \mathbf{N}_u, \sum_I t^{\ell(I)}\hat{S}^I \right\rangle \frac{dt}{t}\,. \tag{17}$$

For u a word of length n, we have therefore to evaluate $\left\langle \mathbf{N}_u, \hat{A}_n(t)\right\rangle$ with $A_n(t) := \sum_{|I|=n} t^{l(I)}S^I$. This last sum is related to a well-known series. The *noncommutative*

Eulerian polynomials are defined by [7, Section 5.4]

$$\mathcal{A}_n(t) = \sum_{k=1}^{n} (\sum_{\substack{|I|=n \\ \ell(I)=k}} R_I) t^k = \sum_{k=1}^{n} \mathbf{A}(n,k)\, t^k. \tag{18}$$

where R_I is the ribbon basis (the basis of **Sym** obtained from the S^I basis by Möbius inversion in the boolean lattice) [7, Section 3.2]. The generating series of the $\mathcal{A}_n(t)$ is given by

$$\mathcal{A}(t) := \sum_{n\geq 0} \mathcal{A}_n(t) = (1-t)\ (1-t\,\sigma_{1-t})^{-1}\ , \tag{19}$$

where $\sigma_{1-t} = \sum (1-t)^n S_n$. Let $\mathcal{A}_n^*(t) = (1-t)^{-n}\,\mathcal{A}_n(t)$. Then,

$$\mathcal{A}^*(t) := \sum_{n\geq 0} \mathcal{A}_n^*(t) = \sum_{I} \left(\frac{t}{1-t}\right)^{\ell(I)} S^I\ . \tag{20}$$

and

$$\sum_{I\vDash n} t^{\ell(I)} S^I = A_n(t) = \mathcal{A}_n^*\left(\frac{t}{1+t}\right) = (1+t)^n \mathcal{A}_n\left(\frac{t}{1+t}\right). \tag{21}$$

To evaluate, for a packed word u of length n, the pairing $\langle \mathbf{N}_u, \hat{A}_n(t)\rangle$, let us start with the observation that, if $u = 1^n$, then, writing $\mathcal{F}_\sigma$ for the dual basis to the $\sigma \in S_n = \mathbf{FQSym}_n$,

$$\Phi_1^\dagger(\mathbf{N}_u) = \frac{1}{n!} \sum_{\sigma\in\mathfrak{S}_n} \mathcal{F}_\sigma, \tag{22}$$

where $\Phi_1^\dagger$ is the adjoint map, so that in this case,

$$\langle \mathbf{N}_u, \hat{A}_n(t)\rangle = \langle \Phi_1^\dagger(\mathbf{N}_u), A_n(t)\rangle = \frac{1}{n!} \sum_{\sigma\in\mathfrak{S}_n} t^{d(\sigma)+1}(1+t)^{r(\sigma)} = \frac{1}{n!} t E_n(t, t+1) \tag{23}$$

where $d(\sigma)$ is the number of descents of σ, $r(\sigma) = n - d(\sigma)$ the number of rises, and E_n is the homogeneous Eulerian polynomial normalized as in [19]

$$E_n(x,y) = \sum_{\sigma\in\mathfrak{S}_n} x^{d(\sigma)} y^{r(\sigma)}\ . \tag{24}$$

Now, recall that the coproduct of $\mathbf{N}_u$ dual to the product of the $\mathbf{M}_u$ is [16]

$$\Delta \mathbf{N}_u = \sum_{u=u_1u_2} \mathbf{N}_{\mathrm{pack}(u_1)} \otimes \mathbf{N}_{\mathrm{pack}(u_2)} \tag{25}$$

(deconcatenation). We can omit the packing operation in this formula if we make the convention that $\mathbf{N}_w = \mathbf{N}_u$ if $u = \mathrm{pack}(w)$. Then, since Φ_1, and hence also $\Phi_1^\dagger$ are morphisms of Hopf algebras, for a composition $L = (l_1, \dots, l_p)$,

$$\langle \Phi_1^\dagger(\mathbf{N}_u), S^L\rangle = \langle \Delta^{[k]}(\mathbf{N}_u), S_{l_1} \otimes ... \otimes S_{l_p}\rangle = \prod_{k=1}^{p} \langle \Phi_1^\dagger(\mathbf{N}_{u_k}), S_{l_k}\rangle \tag{26}$$

where $\Delta^{[k]}$ is the k-th iterated coproduct and $u = u_1u_2\cdots u_p$ with $|u_k| = l_k$ for all k. Moreover, this is nonzero only if all the u_k are nondecreasing, in which case the result is $1/(u_1!\cdots u_p!)$.

Thus, if

$$u = w_1 \cdots w_m \tag{27}$$

is the factorization of u into maximal nondecreasing words, with $|w_k| = n_k$, we have

$$\langle \Phi_1^\dagger(\mathbf{N}_u), A_n(t)\rangle = \prod_{k=1}^{m} \langle \Phi_1^\dagger(\mathbf{N}_{w_k}), A_{n_k}(t)\rangle \tag{28}$$

since

$$\prod_{k=1}^{m} A_{n_k}(t) = \sum_{I\in C_u} t^{\ell(I)} S^I \tag{29}$$

where C_u is the set of compositions which are a refinement of $(n_1, ..., n_m)$ and are the ones such that $\langle \Phi_1^\dagger(\mathbf{N}_u), S^I\rangle \neq 0$.

Next, if $v = 1^{l_1}2^{l_2}\cdots p^{l_p}$,

$$\langle \Phi_1^\dagger(\mathbf{N}_v), S^L\rangle = \prod_{k=1}^{p} \langle \Phi_1^\dagger(\mathbf{N}_{k^{l_k}}), S^{l_k}\rangle \tag{30}$$

(both sides are equal to $1/(l_1!\cdots l_p!)$), so that

$$\langle \Phi_1^\dagger(\mathbf{N}_v), A_{|L|}(t)\rangle = \left(1+\frac{1}{t}\right)^{r(v)} \prod_{k=1}^{p} \langle \Phi_1^\dagger(\mathbf{N}_{k^{l_k}}), A_{l_k}(t)\rangle\,. \tag{31}$$

where $r(v)$ is the number of different letters (or of strict rises) of v. Indeed, $A_{|L|}(t) = \sum_{|I|=|L|} t^{l(I)} S^I$ and, since the S_l are grouplike,

$$\langle \Phi_1^\dagger(\mathbf{N}_u), S^I\rangle = \prod_{k=1}^{p} \langle \Phi_1^\dagger(\mathbf{N}_k^{l_k}), S^{I|k}\rangle,$$

where $I|k$ is the partition of $\{l_1+...+l_{k-1}+1, ..., l_1+....+l_k\}$ induced by the partition I of $[|L|]$. Finally, writing $I\cup L$ for the partition refining I and L (obtained, *e.g.*, by gluing the $I|k$), using

$$\langle \Phi_1^\dagger(\mathbf{N}_u), t^{l(I)}S^I\rangle = t^{l(I)-l(I\cap L)} \langle \Phi_1^\dagger(\mathbf{N}_u), t^{l(I\cap L)} S^{I\cap L}\rangle \tag{32}$$

and noting that $|\{I \models |L|,\ I\cap L = K,\ l(I)-l(K) = k < r(u)\}| = \binom{r(u)}{k}$, we get (31).

We can now see that if we decompose u into maximal blocks of identical letters,

$$u = i_1^{j_1} i_2^{j_2} \cdots i_s^{j_s} \tag{33}$$

we have finally

$$\langle \Phi_1^\dagger(\mathbf{N}_u), A_n(t)\rangle = \left(1+\frac{1}{t}\right)^{r(u)} \prod_{k=1}^{s} \langle \Phi_1^\dagger(\mathbf{N}_{i_k^{j_k}}), A_{j_k}(t)\rangle$$

$$= t^{d(u)+1}(1+t)^{r(u)} \prod_{k=1}^{s} \frac{E_{j_k}(t, 1+t)}{j_k!}$$

which implies Goldberg's formula:

Theorem 25. *The coefficient c_u of $\mathbf{M}_u$ in the Hausdorff series Φ is given by:*

$$c_u = \int_{-1}^{0} t^{d(u)+1}(1+t)^{r(u)} \prod_{k=1}^{s} \frac{E_{j_k}(t, 1+t)}{j_k!} \frac{dt}{t} \tag{34}$$

More generally, for an arbitrary moment generating function

$$f(z) = \sum_{n\geq 1} f_n z^n. \tag{35}$$

with

$$f_n = \int_{\mathcal{R}} t^n d\mu(t) \tag{36}$$

the coefficient of $\mathbf{M}_u$ in $f(\hat{\sigma}_1)$ is

$$\int_{\mathcal{R}} t^{d(u)+1}(1+t)^{r(u)} \prod_{k=1}^{s} \frac{E_{j_k}(t, 1+t)}{j_k!} d\mu(t). \tag{37}$$

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