The Hopf algebra of rooted trees, free Lie algebras, and Lie series

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Abstract

We present, based on our results in [18] where the Hopf algebra structure of the shuffle algebra is described in terms of the Hopf algebra of decorated rooted trees, a rewriting algorithm that provides a simple recursive way to compute the coproduct of the shuffle Hopf algebra in terms of a dual basis of the Poincaré-Birkhoff-Witt basis corresponding to a Hall basis of the free Lie algebra. This can be applied, for instance, to do computations in free Lie algebras and its enveloping associative algebra in terms of an arbitrary Hall basis. In addition, we show how to exploit our results to do algebraic manipulations with Lie series and exponentials of Lie series [20], either using our rewriting algorithm, or working directly in terms of the Hopf algebra of decorated rooted trees. In particular, we give an explicit way to obtain the coefficients of the CBH formula (and also for its continuous version) read directly from the decorated rooted tree associated to each element of the Hall basis.

1 Introduction

Let us fix $\mathbb{Q}$ as the base field. We consider a fixed set D (an alphabet), and denote as $\mathcal{L}(D)$ the free Lie algebra over D. The universal enveloping algebra of $\mathcal{L}(D)$ is canonically isomorphic to the free associative algebra $\mathbb{Q}\langle D\rangle$, or equivalently, the tensor algebra $T(V)$ over $V := \mathrm{span}(D)$, the free $\mathbb{Q}$-module over the set D. Furthermore, $\mathcal{L}(D)$ is canonically isomorphic to the Lie algebra of primitive elements of the bialgebra $T(V)$. This means in particular that the coproduct in $T(V)$ can be used to identify the elements of $\mathcal{L}(D)$ in $T(V)$ [20]. In practice, it is often useful to work in a Poincaré-Birkhoff-Witt basis of $T(V)$ corresponding to some basis of of the free Lie algebra, because in that case, the coproduct in $T(V)$ admits a very simple description (and in particular, provides a direct way of identifying the elements in $\mathcal{L}(D)$), but on the contrary, the explicit description of

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the algebra structure of $T(V)$ becomes more involved. If a (generalized) Hall basis of $\mathcal{L}(D)$ has been chosen, this can be done using some rewriting rule [20].

With the canonical grading of $T(V) = \mathbb{Q} \oplus \bigoplus_{n\geq 1} V^{\otimes n}$, the tensor algebra $T(V)$ has a structure of graded connected cocommutative Hopf algebra. If D is finite, the graded dual of $T(V)$ has a graded connected (actually, strictly graded) commutative Hopf algebra structure denoted by $\mathrm{Sh}(V)$ (here, we identify the linear dual V^* with V). The shuffle algebra $\mathrm{Sh}(V)$ is particularly useful in applications that require dealing with Lie series [20] and exponentials of Lie series. Two such applications are, for instance, non-linear control theory [13], and the theory of geometric numerical integrators for ordinary differential equations [15, 16].

The present work is mainly based on the results in [18], where the Hopf algebra structure of $\mathrm{Sh}(V)$ is described in terms of basis associated to Hall sets of decorated rooted trees, actually, the dual basis of a Poincaré-Birkhoff-Witt basis of $T(V)$ corresponding to a Hall basis of $\mathcal{L}(D)$. The main tool we use is another graded connected commutative Hopf algebra associated to the set D, namely, the commutative Hopf algebra of rooted trees decorated by D, that we denote as $\mathcal{H}_R(V)$, $V := \mathrm{span}(D)$ or simply as $\mathcal{H}_R$.

The commutative Hopf algebra structure $\mathcal{H}_R$ on the vector space spanned the set of (non-decorated) rooted trees was first described by Dür [7], who realized that Butcher's group [3] was actually an affine group scheme, and consequently has associated two dual Hopf algebra structures, a commutative one and a cocommutative one. In [9], the cocommutative dual of $\mathcal{H}_R$ is described together with several other cocommutative Hopf algebras on families of trees including the family of rooted trees decorated by a given set D. Independently, Kreimer [6] rediscovered the Hopf algebra $\mathcal{H}_R$ in the context of renormalization in quantum field theory. Brouder [4] seems to be the first author to note the relationship of Kreimer's work with Butcher's theory.

In [18], an epimorphism ν of graded Hopf algebras from $\mathcal{H}_R(V)$ to $\mathrm{Sh}(V)$ is constructed, and the graded Hopf ideal $\mathcal{I} = \ker \nu$ is explicitly given, showing that $\mathrm{Sh}(V)$ is isomorphic as a graded Hopf algebra to the quotient Hopf algebra $\mathcal{H}_R(V)/\mathcal{I}$. Closely related results can already be found, although not stated in algebraic terms, in [19]. In analogy to Hall set of words (or Hall sets of planar binary trees) [20] Hall sets of decorated rooted trees were first introduced in [19]. In [18], it is shown that the image by $\nu : \mathcal{H}_R(V) \to \mathrm{Sh}(V)$ of an arbitrary Hall set $\widehat{\mathcal{T}}$ of decorated rooted trees freely generates the shuffle algebra $\mathrm{Sh}(V)$, and the Hopf algebra structure of $\mathrm{Sh}(V)$ is completely described in terms of their set of generators $\nu(\widehat{\mathcal{T}})$. Actually, it turns out that the basis $\nu(\widehat{\mathcal{F}})$ of the vector space $\mathrm{Sh}(V)$ obtained as the image by ν of the set of Hall forests $\widehat{\mathcal{F}}$ coincides with the dual of a Poincaré-Birkhoff-Witt basis of $T(V)$ corresponding to a Hall basis of $\mathcal{L}(D)$ [20].

The main goal of the present work is to exploit the results in [18] from a more computational point of view, with special focus to algebraic manipulations with Lie series and exponentials of Lie series [20]. Our results, in particular Algorithm 1 (or alternatively, Algorithm 2) together with recursion (13), can also be useful when doing computations in free Lie algebras $\mathcal{L}(D)$ in terms of Hall basis, and in free associative algebras (that is, tensor algebras over $V = \mathrm{span}(D)$) in terms of a Poincaré-Birkhoff-Witt basis corresponding to a Hall basis of $\mathcal{L}(D)$.

The structure of the rest of the paper is as follows. In Section 2, definitions and fundamental results (together with some useful consequences) on the commutative Hopf algebra of decorated rooted trees are collected. The shuffle Hopf algebra is considered in Section 3, and the relation between the shuffle Hopf algebra $\mathrm{Sh}(V)$ and the Hopf algebra $\mathcal{H}_R(V)$ of decorated rooted trees, explored in [18], is stated (Theorem 1). Section 4 is devoted to describe the Hopf algebra structure of $\mathrm{Sh}(V)$ in terms of a set of free generators of the shuffle algebra. The first four subsections in Section 4 collect several definitions and results from [18] needed in the rest of the paper: Hall sets $\widehat{\mathcal{T}}$ of decorated rooted trees are introduced in Subsection 4.1, and in Subsection 4.2, several results from [18] are collected, where the Hopf algebra structure of $\mathrm{Sh}(V)(V)$ is described in terms of the generator set $\nu(\widehat{\mathcal{T}})$ of its algebra structure. Subsection 4.4 presents some definitions and results of technical nature (also from [18]) which are needed in in Subsection 4.5, where new rewriting algorithms useful to describe the coalgebra structure of $\mathrm{Sh}(V)$ in terms a Hall basis are presented. Finally, Section 5 focuses in exploiting our results to perform algebraic manipulations with Lie series [20] and exponentials of Lie series. Subsection 5.1 and Subsection 5.2 are of introductory nature, where the exponential and the logarithm are considered in a general setting associated to arbitrary commutative graded connected Hopf algebras $\mathcal{H}$. The particular case of $\mathcal{H} = \mathcal{H}_R(V)$ is considered in Subsection 5.3, where explicit formulae are presented for that case. In Subsection 5.4, Lie series, exponentials of Lie series, and the logarithm, are considered with our notation for $\mathcal{H} = \mathrm{Sh}(V)$. Finally, we consider the Campbell-Baker-Hausdorff (CBH) formula and several generalizations in Subsection 5.5 and 5.6. In particular, we give explicit formulae to obtain the coefficients corresponding to the terms of a given Hall basis in the CBH formula and its continuous version.

2 The commutative Hopf algebra of decorated rooted trees

2.1 Rooted trees and forests decorated by D

Given a set D, rooted trees and forests decorated by D can be defined as follows.

A partially ordered set decorated by D is a partially ordered set U together with a map of U onto D (the decoration of U). The elements of U are called vertices. An edge $(x < y)$ of U is an ordered pair $(x, y) \in U \times U$ such that $x < y$ and there exists no $z \in U$ with $x < z < y$. New decorated partially ordered sets can be obtained from U by adding and/or removing some vertices and/or edges.

An isomorphism of partially ordered sets decorated by D is a bijection of the underlying sets that preserves the orderings and the decorations. A forest decorated by D is an isomorphism class of finite partially ordered sets U decorated by D satisfying

$$x, y, z \in U,\ y < x,\ z < x \quad \Longrightarrow \quad \text{either} \ \ y < z \ \ \text{or} \ \ z < y \ \ \text{or} \ \ z = y. \tag{1}$$

The roots of a decorated partially ordered set U representing a decorated forest u are its minimal vertices. A rooted tree decorated by D is a forest represented by decorated partially ordered sets with only one root.

The degree $|u|$ of a forest u decorated by D is the cardinal of the underling set of a representative partially ordered set (that is, the number of vertices in u). Given a forest u decorated by D, the partial degree $|u|_d$ of u with respect to $d \in D$ is the number of vertices in u that are decorated by d. We denote as $\mathcal{F}(D)$ (resp. $\mathcal{T}(D)$) the set of forests (resp. rooted trees) decorated by D, or simply $\mathcal{F}$ (resp. $\mathcal{T}$) if no ambiguity arises. The empty forest is also included in $\mathcal{F}$, and we denote it as e.

We will consider several operations on the set $\mathcal{T}$ of decorated forests. The union of two forests $u, v \in \mathcal{F}$ is the simplest one, and it simply corresponds to the union of two disjoint decorated partially ordered sets representing u and v respectively. We represent the union of u and v simply as uv. The union of forests is obviously associative and commutative. Given $d \in D$, $t_1, \dots, t_m \in \mathcal{T}$, $u = t_1 \cdots t_m \in \mathcal{F}$, we denote by $B_d(u)$ the decorated rooted tree of degree $|t_1| + \cdots + |t_m| + 1$ obtained by grafting the roots of $t_1, \dots, t_m$ to a new root decorated by d. That is, it corresponds to adding a new vertex r to a partially ordered forest U representing u, and adding, for each t_i, a new edge $(r < r_i)$ connecting the root r_i of t_i with r. In particular, $B_d(e)$ is the decorated rooted tree with only one vertex, decorated by d. We hereafter identify $B_d(e)$ with d. Given a decorated rooted tree $t \in \mathcal{T}$ and a decorated forest $u \in \mathcal{F}$, we denote by $u \circ t$ the decorated rooted tree of degree $|u| + |t|$ obtained by grafting the decorated rooted trees in u to the root of t. In particular, $e \circ t = t$ and $u \circ d = B_d(u)$ for $d \in D$, $t \in \mathcal{T}$, $u \in \mathcal{F}$. We also write $e \circ e = e$ and $u \circ e = 0$ for each $u \in \mathcal{F} \backslash \{e\}$.

Given a decorated partially ordered set U representing a decorated forest $u \in \mathcal{F}$, each subset $V = \{x_1, \dots, x_m\}$ of vertices of U determines a new forest $C^V(U)$ of decorated rooted trees obtained by removing all edges of the form $(y < x_i)$, $1 \leq i \leq s$. Note that if x_i is a root of U, then $C^V(U) = C^{V \backslash \{x_i\}}(U)$. If $r_1, \dots, r_l$ are the roots of U that are not in V, then the decorated partially ordered sets representing each decorated rooted tree in $C^V(U)$ have either some r_i $(1 \leq i \leq l)$ or some x_j $(1 \leq j \leq m)$ as its root. We denote as $R^V(U)$ (resp. $P^V(U)$) the forest of the decorated rooted trees in $C^V(U)$ corresponding to $r_1, \dots, r_l$ (resp. $x_1, \dots, x_m$). For $V = \emptyset$, $C^V(U) = R^V(U) = u$ and $P^V(U) = e$. For $V = \{\text{roots of } U\}$, $C^V(U) = P^V(U) = u$ and $R^V(U) = e$.

The symmetry $\sigma(u)$ of a decorated forest u is the number of different bijections of the underlying set of a decorated partially ordered set representing u that are isomorphisms of decorated partially ordered sets.

The symmetry of forests can be recursively obtained as follows.

Lemma 1 *For each $d \in D$, $t_1, \cdots, t_m \in \mathcal{T}$, $t_i \neq t_j$ if $i \neq j$,*

$$\sigma(e) = 1, \quad \sigma(B_d(u)) = \sigma(u), \quad \sigma(u) = \prod_{j=1}^{m} i_j! \sigma(t_j)^{i_j}, \quad \textit{if} \quad u = \prod_{j=1}^{m} t_j^{i_j}.$$

The following definition will be used later on.

Definition 1 *The factorial $u!$ of each forest $u \in \mathcal{F}$ is defined recursively as follows. Given $d \in D$, $t_1, \cdots, t_m \in \mathcal{F}$, $v \in \mathcal{F}$, $t = B_d(v)$, $u = t_1 \cdots t_m$,*

$$d! = 1, \quad t! = v!|t|, \quad u! = t_1! \cdots t_m!.$$

2.2 A Hopf algebra structure of decorated rooted trees

We next describe the commutative Hopf algebra structure on the vector space spanned by the set $\mathcal{F}$ of forests decorated by D [8]. We denote this commutative Hopf algebra structure as $\mathcal{H}_R(V)$, where we write $V = \text{span}(D)$, or simply as $\mathcal{H}_R$ if no ambiguity arises. The product in $\mathcal{H}_R$ corresponds to the union of forests, and the unity element is the empty forest e. As an algebra, $\mathcal{H}_R$ is freely generated by $\mathcal{T}$, i.e., it is the algebra $\mathbb{Q}[\mathcal{T}]$ of polynomials in commuting indeterminates indexed by $\mathcal{T}$. The counit $\epsilon : \mathcal{H}_R \to \mathbb{Q}$ is given by $\epsilon(e) = 1$ and $\epsilon(u) = 0$ for each $u \in \mathcal{F}\backslash\{e\}$. The coproduct $\Delta(u)$ of forest $u \in \mathcal{F}$ is given as follows. For the empty forest $\Delta e = e \otimes e$, and for $u \in \mathcal{F}\backslash\{e\}$, let U be a decorated partially ordered set representing u, then

$$\Delta u = \sum_{V \in R(U)} P^V(U) \otimes R^V(U), \tag{2}$$

where $R(U)$ is a familly of subsets V of U satisfying that

$$x, y \in V, \quad \Longrightarrow \quad y \not< x, \quad x \not< y. \tag{3}$$

In particular, $\Delta d = d \otimes e + e \otimes d$ for each $d \in D$ (that is, all the decorated rooted trees of degree 1 are primitive elements of the Hopf algebra $\mathcal{H}_R$). Note that, for each $t \in \mathcal{T}$, $\Delta t - e \otimes t - t \otimes e$ is a $\mathbb{Z}$-linear combination of terms of the form $u \otimes z$ where $u \in \mathcal{F}\backslash\{e\}$, $z \in \mathcal{T}$, $|u| + |z| = |t|$. It is straightforward to check that $\Delta(uv) = \Delta(u)\Delta(v)$, so that $\Delta : \mathcal{H}_R \to \mathcal{H}_R \otimes \mathcal{H}_R$ is an algebra map. In addition, we have the following. Let us denote as $\mathcal{M}_R$ the linear span of $\mathcal{T}$, and let us consider the left $\mathcal{H}_R$-module structure of $\mathcal{M}_R$ given by the grafting operation $\circ$ extender linearly (clearly, $u \circ t = u' \circ (z \circ t)$ if $u'z = u$, $u' \in \mathcal{F}$, $z \in \mathcal{T}$, $t \in \mathcal{T} \cup \{e\}$). Now, define the $\mathcal{H}_R \otimes \mathcal{H}_R$-module structure of $\mathcal{H}_R \otimes \mathcal{M}_R + \mathcal{M}_R \otimes e$ given by $(u \otimes v) \circ (w \otimes t) = uw \otimes (v \circ t)$ and $(u \otimes v) \circ (t \otimes e) = \epsilon(v) u \circ t \otimes e$, for $u, v, w \in \mathcal{F}$ and $t \in \mathcal{T}$.

Lemma 2 *Given $t \in \mathcal{T}$, $u \in \mathcal{F}$, it holds that*

$$\Delta(u \circ t) = \Delta(u) \circ \Delta(t). \tag{4}$$

Proof: As Δ is an algebra map, and by the left $\mathcal{H}_R$-module (resp. the left $\mathcal{H}_R \otimes \mathcal{H}_R$-module) structure of $\mathcal{M}_R$ (resp. $\mathcal{H}_R \otimes \mathcal{M}_R + \mathcal{M}_R \otimes e$) it is sufficient to prove (4) for $u = z \in \mathcal{T}$. Consider three decorated partially ordered sets T, Z, R representing t, z, and $z \circ t$ respectively. Clearly, each subset V of R satisfying (3) gives rise to two subsets V_1, V_2 of T and Z respectively satisfying (3). Each pair of subsets V_1, V_2 of T and Z satisfying

(3) gives rise to a subset V of R satisfying (3), unless $V_1 = \{r_t\}$ and $V_2 \neq \{r_z\}$, where r_t and r_z are the roots of T and Z respectively. But this exception corresponds to terms of the form $(w \otimes z_1) \circ (t \otimes e)$ $(w \in \mathcal{F},\, z_1 \in \mathcal{T})$ in the right-hand side of (4), which vanish by definition of $\circ$. $\square$

Remark 1 In the particular case of $t = d$, $d \in D$, (4) is equivalent to the identity

$$\Delta(t) = t \otimes e + (\mathrm{id} \otimes B_d)\Delta(u), \quad d \in D, \quad u \in \mathcal{F}, \quad t = B_d(u),$$

given in [6, 8]. $\square$

The Hopf algebra structure $\mathcal{H}_R$ is compatible with the $\mathbb{Z}$-grading induced by the degree $|u|$ of decorated forests. Thus, for each $n \geq 0$, the set $\mathcal{F}_n$ of decorated forests of degree n form a basis of the homogeneous component $(\mathcal{H}_R)_n$. In particular, $(\mathcal{H}_R)_0 = \mathbb{K}e$, and $\mathcal{H}_R$ is a $\mathbb{Z}$-graded connected Hopf algebra. The augmentation ideal $\mathcal{H}_R^+ = \ker \epsilon$ has the set of non-empty forests $\mathcal{F}\backslash\{e\}$ as basis.

As any $\mathbb{Z}$-graded connected bialgebra, the bialgebra $\mathcal{H}_R$ admits a unique $\mathbb{Z}$-graded connected Hopf algebra structure. That is, the antipode S is uniquely determined from the $\mathbb{Z}$-graded algebra structure of $\mathcal{H}_R$ and the definition of the coproduct Δ. Actually, the antipode $S : \mathcal{H}_R \to \mathcal{H}_R$ of $\mathcal{H}_R$ can be given explicitly as follows. Given $t \in \mathcal{T}$, consider a decorated partially ordered set T representing t, and let $r \in T$ be its root, then [6]

$$S(t) = \sum_{Z \in K(T)} (-1)^{|Z|}\, C^Z(T), \tag{5}$$

where $K(T)$ denotes the familly of decorated partially ordered subsets Z of T with the same root as T.

Different universal mapping properties hold for $\mathcal{H}_R$ [6, 8, 18]. The most basic one, that only involves the algebra structure of $\mathcal{H}_R$ and the linear maps $B_d : \mathcal{H}_R \to \mathcal{H}_R$ is as follows.

Proposition 1 *Given a commutative algebra $\mathcal{A}$ and a linear map $L_d : \mathcal{A} \to \mathcal{A}$ for each $d \in D$, there exists a unique algebra map $\phi : \mathcal{H}_R \to \mathcal{A}$ such that $\phi B_d = L_d \phi$ for each $d \in D$.*

3 The shuffle algebra $\mathrm{Sh}(V)$ over V

The shuffle (Hopf) algebra is a commutative graded connected Hopf algebra that can be defined as follows. A commutative algebra structure is given to the vector space $\mathbb{K} \oplus V \oplus V^{\otimes 2} \oplus V^{\otimes 3} \oplus \cdots$ by defining the shuffle product of two *words* as

$$(d_1 \otimes \cdots \otimes d_m)(d_{m+1} \otimes \cdots \otimes d_{m+l}) = \sum d_{i_1} \otimes \cdots \otimes d_{i_{m+l}} \tag{6}$$

where $d_1, \ldots, d_{m+1} \in D$, and the summation goes over all permutations $(i_1, \ldots, i_{m+l})$ of $(1, \ldots, m+l)$ that preserve the partial orderings of $(1, \ldots, m)$ and $(m+1, \ldots, m+l)$. The unity element is the empty word, which we denote as $\widehat{e}$. The degree $|w|$ (resp. partial degree $|w|_d$, $d \in D$) of a word $w = d_1 \otimes \cdots \otimes d_m$ is m (resp. the number of letters in $d_1, \ldots, d_m$ that coincide with d).

As any graded connected algebra, the graded algebra $\mathrm{Sh}(V)$ has a unique augmentation $\widehat{\epsilon} : \mathrm{Sh}(V) \to \mathbb{Q}$ (that is, a unique graded algebra map of $\mathrm{Sh}(V)$ onto $\mathbb{Q}$), which is determined by $\widehat{\epsilon}(\widehat{e}) = 1$ and $\widehat{\epsilon}(w) = 0$ for arbitrary non-empty words w.

The shuffle product satisfies the following identity, that can be used as an alternative recursive definition of the shuffle product (6). Given $d_1, \ldots, d_m \in D$, let us denote $C_{d_1}(\widehat{e}) := d_1$ and $C_{d_m}(d_1 \otimes \cdots \otimes d_{m-1}) := d_1 \otimes d_2 \otimes \cdots \otimes d_m$. Then, each non-empty word can be uniquely written as $C_d(u)$ with $d \in D$ and $u \in \mathrm{Sh}(V)$. It then holds that

$$C_d(u)C_f(v) = C_d(uC_f(v)) + C_f(vC_d(u)), \quad d, f \in D, \quad u, v \in \mathrm{Sh}(V). \tag{7}$$

The augmentation ideal $\mathrm{Sh}(V)^+ = \ker \widehat{\epsilon}$ (that is, the vector space spanned by the set of non-empty words) can be given a left $\mathrm{Sh}(V)$-module structure by setting $w \circ C_d(v) = C_d(wv)$ for each $d \in D$ and $v, w \in \mathrm{Sh}(V)$. In particular, $C_d(w) = w \circ d$ for $d \in D$, $w \in \mathrm{Sh}(V)$. Now, (7) reads $C_d(u)C_f(v) = C_d(u) \circ C_f(v) + C_f(v) \circ C_d(u)$, that is,

$$uv = u \circ v + v \circ u, \quad \text{for each} \quad u, v \in \mathrm{Sh}(V)^+. \tag{8}$$

The definition of $\circ : \mathrm{Sh}(V) \otimes \mathrm{Sh}(V)^+ \to \mathrm{Sh}(V)$ can be extended also to $\mathrm{Sh}(V) \otimes \mathrm{Sh}(V)$ by setting $w \circ \widehat{e} = \widehat{\epsilon}(w)\,\widehat{e}$. Thus, (8) also holds if $u = e$ and $v \in \mathrm{Sh}(V)^+$, but it does not hold if $u = v = \widehat{e}$.

Theorem 1 together with Proposition 1, implies that following universal property of the shuffle algebra [18].

Proposition 2 *If in addition to the assumptions of Proposition 1, it holds that*

$$L_d(a)L_f(b) = L_d(aL_f(b)) + L_f(bL_d(a)), \quad d, f \in D, \quad a, b \in \mathcal{A}, \tag{9}$$

then there exists a unique algebra map $\widehat{\phi} : \mathrm{Sh}(V) \to \mathcal{A}$ *such that* $\widehat{\phi} C_d = L_d \widehat{\phi}$ *for each* $d \in D$*. Moreover, it holds that* $\phi = \widehat{\phi}\nu$*, where* $\phi : \mathcal{H}_R \to \mathcal{A}$ *is the algebra map given by Proposition 1.*

Proposition 2 implies the following [18].

Corollary 1 *Given a commutative algebra* $\mathcal{A}$*, a vector subspace* $\mathcal{M}$ *of* $\mathcal{A}$ *with a left* $\mathcal{A}$*-module structure* $\circ : \mathcal{A} \otimes \mathcal{M} \to \mathcal{M}$ *satisfying*

$$mm' = m \circ m' + m' \circ m, \quad m, m' \in \mathcal{M}, \tag{10}$$

and a map $l : D \to \mathcal{M}$*, then there exists a unique algebra map* $\widehat{\phi} : \mathrm{Sh}(V) \to \mathcal{A}$ *such that,* $\widehat{\phi}(d) = l(d)$ *for* $d \in D$ *and* $\widehat{\phi}(w_1 \circ w_2) = \widehat{\phi}(w_1) \circ \widehat{\phi}(w_2)$ *for each* $w_1 \in \mathrm{Sh}(V)$*,* $w_2 \in \mathrm{Sh}(V)^+$*.*

Remark 2 The vector space $\mathrm{Sh}(V)$ has with $\circ : \mathrm{Sh}(V)\otimes\mathrm{Sh}(V) \to \mathrm{Sh}(V)$ a non-associative algebra structure that is sometimes called chronological algebra (see [11] and references therein). Corollary 1 is closely related to the fact that the chronological algebra $\mathrm{Sh}(V)$ is free over the set D [11]. In [21], the term of Zinbiel algebra is used instead, while the term chronological algebra is reserved for a different (although related) non-associative algebra structure introduced in [1]. □

The commutative graded connected algebra $\mathrm{Sh}(V)$ is endowed with a unique graded (commutative and connected) Hopf algebra structure by defining the coproduct $\widehat{\Delta} : \mathrm{Sh}(V) \to \mathrm{Sh}(V) \otimes \mathrm{Sh}(V)$ as below.

In order to avoid confusion, we will denote in what follows each word $d_1 \otimes \cdots \otimes d_m$ as $(d_1 \top \cdots \top d_m)$. More generally, given two words $u = (d_1 \top \cdots \top d_m)$ and $v = (d_{m+1} \top \cdots \top d_{m+n})$ we define the concatenation $w = u \top v$ as the new word $w = (d_1 \top \cdots \top d_{m+n})$. We also define $u \top \widehat{e} = \widehat{e} \top u = u$.

Now, we can define the coproduct $\widehat{\Delta} u$ of each word w as

$$\Delta u = \sum_{u = v \top w} v \otimes w, \tag{11}$$

where the summation is over all pairs of words (v, w) (including the empty word $\widehat{e}$) such that $v \top w = u$.

It is straightforward to check that the following holds for the coproduct $\widehat{\Delta}$ in $\mathrm{Sh}(V)$. Given $w \in \mathrm{Sh}(V)^+$, let $d \in D$ and $v \in \mathrm{Sh}(V)$ be such that $w = C_d(v) = v \top d$, then

$$\widehat{\Delta}(w) = w \otimes \widehat{e} + (\widehat{\mathrm{id}} \otimes C_d)\widehat{\Delta}(v). \tag{12}$$

Clearly, (12) recursively determines the coproduct of $w \in \mathrm{Sh}(V)^+$. An identity analogous to (4) (that can also be used to recursively determine $\widehat{\Delta}(w)$ for $w \in \mathrm{Sh}(V)^+$), can be obtained from (12) as follows. Consider, given $v_1, v_2, w_1 \in \mathrm{Sh}(V)$, $w_1 \in \mathrm{Sh}(V)^+$,

$$\begin{aligned} (v_1 \otimes v_2) \circ (w_1 \otimes w_2) &= v_1 w_1 \otimes (v_2 \circ w_2), \\ (v_1 \otimes v_2) \circ (w_1 \otimes \widehat{e}) &= v_1 \circ w_1 \otimes v_2 \circ \widehat{e} = \widehat{\epsilon}(v_2) v_1 \circ w_1 \otimes \widehat{e}. \end{aligned}$$

This gives a left $\mathrm{Sh}(V) \otimes \mathrm{Sh}(V)$-module structure to $\mathrm{Sh}(V) \otimes \mathrm{Sh}(V)$. Then, (12) implies that

$$\widehat{\Delta}(w \circ v) = \widehat{\Delta}(w) \circ \widehat{\Delta}(v), \quad w, v \in \mathrm{Sh}(V). \tag{13}$$

The relation between the Hopf algebras $\mathrm{Sh}(V)$ and $\mathcal{H}_R(V)$ can be stated as follows [18].

Theorem 1 *There exists a unique algebra map $\nu : \mathcal{H}_R(V) \to \mathrm{Sh}(V)$ such that $\nu(d) = d$ and $\nu(u \circ t) = \nu(u) \circ \nu(t)$ for each $d \in D$, $u \in \mathcal{H}_R(V)$, $t \in \mathcal{M}_R$. Moreover, ν is an epimorphism of graded Hopf algebras. The graded Hopf algebra $\mathrm{Sh}(V)$ is isomorphic to the* *graded quotient Hopf algebra $\mathcal{H}_R(V)/\mathcal{I}$, where $\mathcal{I} = \ker \nu$ is the graded ideal generated by* $\mathrm{Im}\,(\xi - \mathrm{id})$, *where $\xi : \mathcal{H}_R^+ \to \mathcal{M}_R$ is the linear map given by*

$$\xi(t_1 \cdots t_m) = \sum_{i=1}^{m} (t_1 \cdots t_{i-1} t_{i+1} \cdots t_m) \circ t_i, \quad t_1, \ldots, t_m \in \mathcal{T}, \quad m > 1, \tag{14}$$

and $\xi(t) = t$ if $t \in \mathcal{T}$.

Remark 3 Clearly, it holds that $\nu B_d = C_d \nu$ for each $d \in D$. This implies that

$$\nu(B_{d_1} \cdots B_{d_{m-1}}(d_m)) = (d_1 \top \cdots \top d_m), \; m \geq 1, \; d_1, \ldots, d_m \in D, \tag{15}$$

which provides a bijection between the set of non-empty words and the set of decorated rooted trees without ramifications. □

Remark 4 Let us denote $\mathcal{S}_m = \{\xi(t_1 \cdots t_m) - t_1 \cdots t_m : \; t_1, \ldots, t_m \in \mathcal{M}_R\}$ for each $m \geq 1$. It is not difficult to check that $\mathcal{I} = \ker \nu$ (the ideal generated by $\mathrm{Im}\,(\mathrm{id} - \xi) = \sum_{m \geq 2} \mathcal{S}_m$) is actually generated by the set $\mathcal{S}_2 \cup \mathcal{S}_3$, or alternatively, by the set $\mathcal{S}_2 \cup (\mathcal{S}_2 \circ \mathcal{M}_R)$. □

4 The shuffle algebra and Hall sets of rooted trees

4.1 Hall sets of rooted trees

Given a subset $\widehat{\mathcal{T}}$ of the set $\mathcal{T}$ of rooted trees decorated by D, we consider the set of forests $u = t_1 \cdots t_m$, where $t_1, \ldots, t_m \in \widehat{\mathcal{T}}$. We denote by $\widehat{\mathcal{F}}$ the set of such forests, including the empty forest e, and we denote as $\widetilde{\mathcal{T}}$ the subset of decorated rooted trees of the form $B_d(u)$, $d \in D$, $u \in \widehat{\mathcal{F}}$.

If $\widehat{\mathcal{T}}$ has a total order relation, we give a total ordering to $\widehat{\mathcal{T}} \cup \{e\}$ by considering $e < t$ for each $t \in \widehat{\mathcal{T}}$. If $u = t_1 \cdots t_m \in \widehat{\mathcal{F}}$, we define $\min(u) = \min(t_1, \ldots, t_m)$, $\max(u) = \max(t_1, \ldots, t_m)$, $\min(e) = e$, and $\max(e) = e$.

Definition 2 *A subset $\widehat{\mathcal{T}} \subset \mathcal{T}$ is* consistent *if the following condition holds. Given $t_1, \ldots, t_m \in \mathcal{T}$, $d \in D$, if $B_d(t_1 \cdots t_m) \in \widehat{\mathcal{T}}$, then $d, t_1, \ldots, t_m \in \widehat{\mathcal{T}}$.*

Definition 3 *Given a totally ordered consistent subset $\widehat{\mathcal{T}}$ of $\mathcal{T}$, and the corresponding set $\widetilde{\mathcal{T}} := \bigcup_{d \in D} B_d(\widehat{\mathcal{F}})$, the* standard decomposition *(t', t'') of each $t \in \widetilde{\mathcal{T}}$ is defined as follows. If $|t| = 1$, then $t' = t$ and $t'' = e$. If $t = B_d(t_1 \cdots t_m)$, $d \in D$, $t_1, \ldots, t_m \in \widehat{\mathcal{T}}$, $t_1 \leq \cdots \leq t_m$, then $t'' = t_m$, $t' = B_d(t_1 \cdots t_{m-1})$.*

Definition 4 *We say that a consistent set $\widehat{\mathcal{T}} \subset \mathcal{T}$ supplied with a total ordering $<$ is a* Hall set *of rooted trees decorated by D (or simply a Hall set of rooted trees, if D is clear from the context), if $D \subset \widehat{\mathcal{T}}$ and the following condition holds.*

$$t, z \in \widehat{\mathcal{T}}, \quad t > z \geq t'' \quad \Longrightarrow \quad z \circ t \in \widehat{\mathcal{T}}, \quad z \circ t > z. \tag{16}$$

If in addition $t > t'$ for each $t \in \widehat{\mathcal{T}}$ of degree $|t| > 1$, then we say that $(\widehat{\mathcal{T}}, <)$ is a special Hall set *of rooted trees decorated by D.*

Remark 5 Condition (16) can be rewritten as follows. Given $t \in \widetilde{\mathcal{T}}$ of degree $|t| > 1$, let (t', t'') be the standard decomposition of t. If $t' \in \widehat{\mathcal{T}}$ and $t' > t''$ then $t \in \widehat{\mathcal{T}}$ and $t > t''$ (and $t > t'$ if $\widehat{\mathcal{T}}$ is a special Hall set). $\square$

Remark 6 If $\widehat{\mathcal{T}}$ is a special Hall set of rooted trees, and $t_1, \ldots, t_m, z \in \widehat{\mathcal{T}}$ and $z > \max(t_1 \cdots t_m)$, then $(z^k t_1 \cdots t_m) \circ z \in \widehat{\mathcal{T}}$ for each $k \geq 1$. If $\widehat{\mathcal{T}}$ is a Hall set satisfying that for each $t, z \in \widehat{\mathcal{T}}$,

$$|t| < |z| \quad \Longrightarrow \quad t < z, \tag{17}$$

then $\widehat{\mathcal{T}}$ is a special Hall set, and

$$\widehat{\mathcal{T}} = D \cup \{z \circ t : \ t, z \in \widehat{\mathcal{T}}, \ t > z\}. \tag{18}$$

In fact, this is true if the ordering of $\mathcal{T}$ is compatible with any $\mathbb{Z}$-grading of $V = \mathbb{K}D$.

If $\mathcal{T}$ is provided with a total ordering $<$ satisfying (17) (or the corresponding compatibility relation with an arbitrary $\mathbb{Z}$-grading of $V = \mathrm{span}(D)$), then there is a unique Hall set $\widehat{\mathcal{T}}$ of rooted trees decorated by D whose total ordering is inherited from that of $\mathcal{T}$, namely, the special Hall set given by (18). $\square$

Remark 7 Given a Hall set H of words over the alphabet D [20], a Hall set $\widehat{\mathcal{T}}$ of rooted trees decorated by D can be obtained as the image of a map $r : H \to \mathcal{T}$ from the set of Hall words H to the set of decorated rooted trees defined as follows. For $d \in D \subset H$, set $r(d) = d$. For a Hall word $w \in H$ of degree $|w| > 1$, let $d \in D$ be the rightmost letter in w, so that $w = v \top d$ (that is, $w = C_d(v)$), where v is a (non-necessarily Hall) word. It is a standard result [20] that there exists a unique non-decreasing decomposition of v in Hall words, that is, $v = w_m \top \cdots \top w_1$, where $w_1, \ldots, w_m \in H$ are Hall words satisfying that $w_m \geq \cdots \geq w_1$. Then, we set $t = r(w) = B_d(r(w_1) \cdots r(w_m))$. Conversely, given a Hall rooted tree $t = B_d(t_1 \cdots t_m) \in \widehat{\mathcal{T}}$ of degree $|t| > 1$, where $d \in D$, $t_1, \ldots, t_m \in \widehat{\mathcal{T}}$, $t_1 \leq \cdots \leq t_m$, then the corresponding Hall word is $w = r^{-1}(t) = r^{-1}(t_m) \top \cdots \top r^{-1}(t_1) \top d$. We thus have that $r(w) = r(w'') \circ r(w')$ if $w = w'' \top w'$ is the standard factorization of the Hall word $w \in H$, and $r^{-1}(t) = r^{-1}(t'') \top r^{-1}(t')$ if (t', t'') is the standard decomposition of the Hall rooted tree $t \in \widehat{\mathcal{T}}$. Note that, compared to [20], we have reversed the left and right factors in the concatenation product of words, and also the role of the total order relation $<$ on H. $\square$

4.2 Hall basis of the shuffle algebra over V

Hereafter, $\widehat{\mathcal{T}}$ will denote a given Hall set of rooted trees decorated by D, and $\widehat{\mathcal{F}}$ will be the corresponding set of Hall forests. Let us denote $\widehat{\mathcal{H}}_R = \mathbb{K}[\widehat{\mathcal{T}}]$ the subalgebra of $\mathcal{H}_R$ generated by $\widehat{\mathcal{T}}$, which is a commutative graded connected algebra. Clearly, the set $\widehat{\mathcal{F}} \backslash \{e\}$ of non-empty Hall forests is a basis of its augmentation ideal $\widehat{\mathcal{H}}_R^+ = \bigoplus_{n \geq 1} (\widehat{\mathcal{H}}_R)_n$.

The proof of following results (Subsections 4.2–4.4) can be found in [18]. Theorems 2 and 3 below were originally given with different approach and notation in [22, 17, 20].

Theorem 2 *As a graded algebra,* $\mathrm{Sh}(V)$ *is freely generated by the set* $\{\nu(t) : t \in \widehat{\mathcal{T}}\}$, *where* $\nu : \mathcal{H}_R(V) \to \mathrm{Sh}(V)$ *is the unique graded Hopf algebra homomorphism given by Theorem 1.*

Remark 8 Theorem 2 implies that $\nu(\widehat{\mathcal{F}}) = \{\nu(u) : u \in \widehat{\mathcal{F}}\}$ is a basis of the vector space $\mathrm{Sh}(V)$, so that each word $w = d_1 \top \cdots \top d_m$ in $\mathrm{Sh}(V)$ ($d_i \in D$) can be written uniquely as a $\mathbb{Q}$-linear combination of elements in the basis $\nu(\widehat{\mathcal{F}})$. Actually, each word is written as a $\mathbb{Z}$-linear combination of terms of the form $\nu(u)/\sigma(u)$, $u \in \widehat{\mathcal{F}}$. In [18], it is shown that a new forest u^* can be found for each $u \in \widehat{\mathcal{F}}$ such that $\nu(u^*) = \nu(u)/\sigma(u)$, and that $\{\nu(u^*) : u \in \widehat{\mathcal{F}}\}$ is a $\mathbb{Z}$-basis of $\mathrm{Sh}(V)$. □

Remark 9 A complete description of the coalgebra structure is given, according to Theorem 1, by the identity

$$\widehat{\Delta}\nu = (\nu \otimes \nu)\Delta, \tag{19}$$

that is,

$$\widehat{\Delta}\nu(u) = \sum_{V \in R(U)} \nu(P^S(U)) \otimes \nu(R^S(U)), \quad u \in \widehat{\mathcal{T}}, \tag{20}$$

where $R(U)$ is the familly of subsets S of a decorated partially ordered set U representing u that satisfy (3). It can be seen that, $P^V(U) \in \widehat{\mathcal{F}}$ in (20), but in general $R^V(U) \notin \widehat{\mathcal{F}}$. If it is required to express $\widehat{\Delta}(\nu(u))$ in the basis $\{\nu(v_1)\otimes\nu(v_2) : v_1, v_2 \in \widehat{\mathcal{F}}\}$, one of the options is to rewrite each $\nu(R^V(U))$ in (20), in the basis $\nu(\widehat{\mathcal{F}})$. Each $\nu(t)$ with $t \in \mathcal{T}\backslash\widehat{\mathcal{T}}$ can be rewritten in terms of the basis $\nu(\widehat{\mathcal{F}})$ in a recursive way if one has an explicit description of the linear maps $C_d : \mathrm{Sh}(V) \to \mathrm{Sh}(V)^+$ in terms of the basis $\nu(\widehat{\mathcal{F}})$. One just need to consider $d \in D$, $z_1, \ldots, z_m \in \widehat{\mathcal{T}}$ such that $t = B_d(z_1 \cdots z_m)$, rewrite each z_i, and take into account that $\nu B_d = C_d \nu$. An alternative for expressing $\widehat{\Delta}(\nu(u))$ in the basis $\{\nu(v_1) \otimes \nu(v_2) : v_1, v_2 \in \widehat{\mathcal{F}}\}$ is to apply recursively (12), so that we again need the explicit description of the maps $C_d : \mathrm{Sh}(V) \to \mathrm{Sh}(V)^+$ in terms of the basis $\nu(\widehat{\mathcal{F}})$. □

Lemma 3 *The restriction* $\widehat{\xi} : \widehat{\mathcal{H}}_R^+ \to \bigoplus_{d\in D} B_d(\widehat{\mathcal{H}}_R)$ *to the map* ξ *given in Theorem 1 is an isomorphism of graded vector spaces.*

Proposition 3 *Given* $w, v \in \widehat{\mathcal{F}}$, $d \in D$,

$$C_d(\nu(u)) = \nu(\widehat{\xi}^{-1} B_d(u)), \quad \nu(u) \circ \nu(v) = \nu(\widehat{\xi}^{-1}(u \circ \widehat{\xi}(v))). \tag{21}$$

4.3 The dual basis of $\nu(\widehat{\mathcal{F}})$

Let us now consider the dual algebra $\mathrm{Sh}(V)^*$ of the coalgebra structure of $\mathrm{Sh}(V)$. That is, as a vector space, $\mathrm{Sh}(V)^*$ is the linear dual of $\mathrm{Sh}(V)$, the unit in $\mathrm{Sh}(V)^*$ is the counit $\widehat{\epsilon}$ of $\mathrm{Sh}(V)$, and for each $\alpha, \beta \in \mathrm{Sh}(V)^*$, the product $\alpha\beta$ is defined by

$$\langle \alpha\beta, w\rangle = \langle \alpha \otimes \beta, \widehat{\Delta} w\rangle, \quad w \in \mathrm{Sh}(V). \tag{22}$$

Recall that the subalgebra of $\mathrm{Sh}(V)^*$ of linear forms α such that $\langle \alpha, w\rangle \neq 0$ for a finite number of words w is isomorphic to the tensor algebra $T(V)$.

We now consider the dual basis of the basis $\{\nu(u)/\sigma(u) : \ u \in \widehat{\mathcal{F}}\}$ of $\mathrm{Sh}(V)$, which is a basis of the underlying vector space of the tensor algebra $T(V)$ defined as follows. We hereafter denote $\psi(u) = \nu(u)/\sigma(u)$ for each $u \in \widehat{\mathcal{F}}$ (that is, following Remark 8, $\psi(u) = \nu(u^*)$).

Definition 5 *For each $u \in \widehat{\mathcal{F}}\backslash\{e\}$, we define $F_u \in \mathrm{Sh}(V)^*$ such that, given $v \in \widehat{\mathcal{F}}$, $\langle\ F_u, \psi(v)\ \rangle$ is equal to 1 if $u = v$ and 0 otherwise.*

The following theorem states that $\{F_t : \ t \in \widehat{\mathcal{T}}\}$ is the Hall basis [20] of the free Lie algebra $\mathcal{L}(D)$ over D associated to the Hall set $\widehat{\mathcal{T}}$, and that the dual basis $\{F_u : \ u \in \widehat{\mathcal{F}}\}$ of $\psi(\widehat{\mathcal{F}}) = \{\psi(u) : \ u \in \widehat{\mathcal{F}}\}$ is the Poincaré-Witt-Birkhoff basis of $T(V)$ corresponding to the basis $\{F_t : \ t \in \widehat{\mathcal{T}}\}$ of $\mathcal{L}(D)$.

Theorem 3 *Let us assume that $\widehat{\mathcal{T}}$ is a Hall set of rooted trees decorated by D. Given an arbitrary $t \in \widehat{\mathcal{T}}$ with $|t| > 1$. Let (t', t'') be the standard decomposition of the Hall rooted tree t, then it holds that*

$$F_t = [F_{t''}, F_{t'}]. \tag{23}$$

Furthermore, for arbitrary $t_1, \ldots, t_m \in \widehat{\mathcal{T}}$ such that $t_1 \leq \cdots \leq t_m$, it holds that

$$F_u = F_{t_m} \cdots F_{t_1}, \quad \text{for} \quad u = t_1 \cdots t_m. \tag{24}$$

4.4 Auxiliary definitions and results on Hall rooted trees

Let us denote $\widetilde{\mathcal{T}} := \bigcup_{d\in D} B_d(\widehat{\mathcal{F}})$, and for each $t \in \widetilde{\mathcal{T}}$ of degree $|t| > 1$, we consider the standard decomposition $(t', t'') \in \widetilde{\mathcal{T}} \times \widehat{\mathcal{T}}$.

Definition 6 *We define the map $\Gamma : \widehat{\mathcal{F}}\backslash\{e\} \to \widetilde{\mathcal{T}}$ given as follows. Given $u \in \widehat{\mathcal{F}}\backslash\{e\}$, if $u \in \widehat{\mathcal{T}}$, we set $\Gamma(u) = u$, and if $u \notin \widehat{\mathcal{T}}$, we define $\Gamma(u) = v \circ t$ such that $t \in \widehat{\mathcal{T}}$, $v \in \widehat{\mathcal{F}}$, $u = tv$ and $t \leq \min(v)$.*

Lemma 4 *The map Γ is bijective, and for each $t \in \widetilde{\mathcal{T}}$, it holds that $\Gamma^{-1}(t) = t$ if $t \in \widehat{\mathcal{T}}$ and $\Gamma^{-1}(t) = t''\Gamma^{-1}(t')$ otherwise.*

Remark 10 Lemma 4 gives a convenient way of obtaining the values $\Gamma^{-1}(t)$ for $t \in \widetilde{\mathcal{T}}$ in a recursive way. □

Definition 7 *For each $u \in \widehat{\mathcal{F}}\backslash\{e\}$, we define a set $S_u \subset \widehat{\mathcal{F}}$ of Hall forests as follows. Let $t_0, \ldots, t_m \in \widehat{\mathcal{T}}$, $k_0, \ldots, k_m \geq 1$ be such that $t_0 < \cdots < t_m$ and $u = t_0^{k_0} \cdots t_m^{k_m}$. Let us consider for each $i = 0, \ldots, m$ the Hall forests $u_i, v_i \in \widehat{\mathcal{F}}$ such that $u = u_i t_i$ and $v_i = \Gamma^{-1}(u_i \circ t_i)$. (In particular, we have by definition of Γ that $v_0 = u$.) Then, we define $S_u = \{v_1, \ldots, v_m\}$, and denote $\mu(u, u) = -1/k_0$ and $\mu(u, v_i) = -k_i/k_0$ for $i = 1, \ldots, m$.*

Lemma 5 *Given $u, v \in \widehat{\mathcal{F}}\backslash\{e\}$ such that $v \in S_u$, let $t = \min(v)$. It holds that $\min(u) \leq t'' < t$ and $\max(v) \leq \max(u)$, $|\min(u)| < |\min(v)|$, and $|\min(u)|_d \leq |\min(v)|_d$ and $|u|_d = |v|_d$ for each $d \in D$.*

Definition 8 *Given $u, v \in \widehat{\mathcal{F}}\backslash\{e\}$, a path of length m from u to v is a finite sequence $W = (w_0, \ldots, w_m)$ such that $m \geq 0$, $w_0, \ldots, w_m \in \widehat{\mathcal{F}}\backslash\{e\}$, $w_0 = u$, $w_m = v$ and $w_{j+1} \in S_{w_j}$, $0 \leq j \leq m-1$. In such case, we write*

$$\mu(W) = \prod_{j=0}^{m-1} \mu(w_j, w_{j+1}).$$

We define a partial order $\succ$ in $\widehat{\mathcal{F}}\backslash\{e\}$ as follows. Given $u, v \in \widehat{\mathcal{F}}\backslash\{e\}$, we write $u \succ v$ if there exists some path from u to v. In such case, we denote $\mu(u,v) = \sum_W \mu(W)$ where the summation is over all paths from u to v. For each $u \in \widehat{\mathcal{F}}\backslash\{e\}$ we denote $\overline{S}_u = \{v \in \widehat{\mathcal{F}}\backslash\{e\} : \ u \succ v\}$.

Remark 11 Lemma 5 implies that $\min(u) < \min(v) \leq \max(v) \leq \max(u)$ provided that $u \succ v$. Hence, $\succ$ is a well defined partial order on $\widehat{\mathcal{F}}\backslash\{e\}$. Moreover, if $u \succ v$, then $|u|_d = |v|_d$ for each $d \in D$. As the sets of forests with same partial degrees are finite, the connected components of $\widehat{\mathcal{F}}\backslash\{e\}$ with respect to the partial order $\succ$ are finite (actually, with the partial order $\succ$, the connected components represent finite oriented graphs). In particular, $\overline{S}_u$ is finite for each $u \in \widehat{\mathcal{F}}\backslash\{e\}$. $\square$

Remark 12 Lemma 5 implies that the maximal length of paths starting from a given $u \in \widehat{\mathcal{F}}$ can be bounded by $|u| - |\min(u)|$ (this upper bound is not optimal). If $\widehat{\mathcal{T}}$ is a special set of Hall rooted trees, then such maximal length for a forest $u = t_1^{k_1} \cdots t_m^{k_m}$ $(t_1, \ldots, t_m \in \widehat{\mathcal{T}})$ can be bounded by $m-1$. $\square$

Lemma 6 *Consider the inverse $\widehat{\xi}^{-1}$ of the restriction $\widehat{\xi} : \widehat{\mathcal{H}}_R^+ \to \bigoplus_{d \in D} B_d(\widehat{\mathcal{H}}_R)$ to the linear map ξ given in Theorem 1. For each $u \in \widehat{\mathcal{F}}$,*

$$\widehat{\xi}^{-1}(\Gamma(u)) = \mu(u,v)\, u + \sum_{v \in \overline{S}_u} \mu(u,v)\, v. \tag{25}$$

Proposition 4 *Given $w \in \widehat{\mathcal{F}}$, $d \in D$, If $\Gamma^{-1}(B_d(w)) = u \in \widehat{\mathcal{F}}$, then*

$$C_d(\nu(w)) = \mu(u,u)\nu(u) + \sum_{v \in \overline{S}_u} \mu(u,v)\nu(v). \tag{26}$$

Lemma 7 *Given $u, v \in \widehat{\mathcal{F}}$, $\nu(u) \circ \nu(v)$ is a $\mathbb{Q}$-linear combination of $\nu(uv)$ and terms of the form $\nu(w)$, $w \in \overline{S}_{uv}$.*

4.5 Rewriting algorithms

The following provides algorithms that can be used to rewrite each $\nu(u)\circ\nu(v)$, $u, v \in \widehat{\mathcal{F}}\backslash\{e\}$ recursively in the basis $\nu(\widehat{\mathcal{F}})$ of $\mathrm{Sh}(V)$ without making explicit use of Lemma 7.

Definition 9 *We consider the subset of $\widehat{\mathcal{F}}\times\widehat{\mathcal{F}}$ defined as*

$$\mathcal{S} = \{(u,v):\ u,v \notin \widehat{\mathcal{T}},\ \max(u) \geq \max(v)\} \cup \{(u,t^k):\ u \notin \widehat{\mathcal{T}},\ t \in \widehat{\mathcal{T}},\ \max(u) > t\}, \tag{27}$$

and define a partial order $>$ on $\widehat{\mathcal{F}}\times\widehat{\mathcal{F}}$ as the completion of the following relations. Let $t, z \in \widehat{\mathcal{T}}$, and $u, v, w, w_1, w_2 \in \widehat{\mathcal{F}}\backslash\{e\}$,

$$t > z \implies (t,z) > (z,t), \tag{28}$$
$$v \notin \widehat{\mathcal{T}} \implies (t,v) > (v,t), \tag{29}$$
$$uv \succ w_1w_2 \implies (u,v) > (w_1,w_2), \tag{30}$$
$$u,v \notin \widehat{\mathcal{T}} \text{ and } \max(u) < \max(v) \implies (u,v) > (v,u), \tag{31}$$
$$\min(w) \geq \max(uv) \implies (wu,v) > (w,uv). \tag{32}$$

Lemma 8 *If $(u,v)\in\mathcal{S}$ then there exist $w_1, w_2 \in \widehat{\mathcal{F}}\backslash\{e\}$ such that*

$$u = w_1w_2 \text{ and, } \ \text{if } w \preceq w_2v, \ \text{then } (u,v) > (w_1,w). \tag{33}$$

Proof: By definition of $\mathcal{S}$ and the partial order relation on $\widehat{\mathcal{F}}\times\widehat{\mathcal{F}}$, it is sufficient to choose $w_1, w_2 \in \widehat{\mathcal{F}}\backslash\{e\}$ such that $u = w_1w_2$ and $\min(w_1) \geq \max(w_2v)$. Clearly, this is always possible, in particular, one can choose $w_1 = t = \max(u)$ or also $w_1 = t^k$ such that $u = t^kw_2$ with $t > \max(w_2)$. $\square$

Algorithm 1 Given $u, v \in \widehat{\mathcal{F}}\backslash\{e\}$,

1. If $u = w^k$, $v = w^l$, where $k, l \geq 1$ and $w \in \widehat{\mathcal{F}}\backslash\{e\}$, then

$$\nu(u)\circ\nu(v) := \frac{l}{k+l}\nu(w^{k+l}),$$

2. Otherwise, if $(u,v) > (v,u)$ then

$$\nu(u)\circ\nu(v) := \nu(uv) - \nu(v)\circ\nu(u),$$

3. Otherwise, if $(u,v)\in\mathcal{S}$, then, choose $w_1, w_2 \in \widehat{\mathcal{F}}\backslash\{e\}$ such that (33) holds, and

$$\nu(u)\circ\nu(v) := \nu(w_1)\circ(\nu(w_2)\circ\nu(v)),$$

4. Otherwise, we have that $v = t^k$, $k \geq 1$, $t \in \widehat{\mathcal{T}}$, and then

$$\nu(u)\circ\nu(v) := k\,\nu(w)\circ\nu(z),$$

   where $w \in \widehat{\mathcal{F}}$ and $z \in \widehat{\mathcal{T}}$ are such that $(t^{k-1}u)\circ t = w\circ z = \Gamma(wz)$, and Γ is given in Definition 6

Remark 13 By definition of $\mathcal{S}$, in Step 4 in Algorithm 1, it always holds that $u = t^k$, $t \in \widehat{\mathcal{T}}$, $k \geq 1$, and $\max(u) \leq t$. The resulting algorithm is particularly convenient when $\widehat{\mathcal{T}}$ is a special Hall set of rooted trees, because $(t^{k-1}u) \circ t \in \widehat{\mathcal{T}}$ if $t \geq \max(v)$, so that Step 4 of Algorithm 1 requires no recursion (that is, Step 4 always gives $w = e$). □

We will verify our rewriting algorithm by considering Algorithm 1 for an arbitrary set $\mathcal{S}$ and a partial order relation on $\widehat{\mathcal{F}} \times \widehat{\mathcal{F}}$ satisfying the following assumptions.

Assumption 1 *There is a partial order relation $<$ on the set of pairs (u, v), $u, v \in \widehat{\mathcal{F}} \backslash \{e\}$ and a set $\mathcal{S} \subset \{(u, v) : \ u, v \in \widehat{\mathcal{F}} \backslash \{e\}, \ u \notin \mathcal{T}, \ (u, v) \not> (v, u)\}$ satisfying the following conditions. Let $t, z \in \widehat{\mathcal{T}}$, and $u, v, w, w_1, w_2 \in \widehat{\mathcal{F}} \backslash \{e\}$,*

1. *If $(u, v) \not> (v, u)$, then either (i) $(u, v) \in \mathcal{S}$, or (ii) $v = t^k$, $t \in \widehat{\mathcal{T}}$, $k \geq 1$, and $\min(u) < t$, or (iii) there exist $w \in \widehat{\mathcal{F}} \backslash \{e\}$ and $k, l \geq 1$ such that $u = w^k$, $v = w^l$.*

2. *If $(u, v) \in \mathcal{S}$ then there exist $w_1, w_2 \in \widehat{\mathcal{F}} \backslash \{e\}$ such that (33) holds.*

3. *If $uv \succ w_1 w_2$, then $(u, v) > (w_1, w_2)$*

4. *For each $u, v \in \widehat{\mathcal{F}} \backslash \{e\}$, the set of pairs (w_1, w_2) such that $(u, v) > (w_1, w_2)$ is finite,*

Remark 14 Conditions 1 and 3 hold by Definition 9, and Lemma 8 precisely states that condition 2 hold. As for condition 4, it follows from the observation that, given a pair (u, v), only a finite number of pairs (w_1, w_2) satisfy each of the conditions (28)–(32) giving the relation $(u, v) > (w_1, w_2)$ without applying the transitivity of the relation $>$ (recall that, according to Remark 11, the set $\overline{S}_u = \{v \in \widehat{\mathcal{F}} : u \succ v\}$ is finite). □

Proposition 5 *Under Assumption 1, Algorithm 1 can be used to express, in a finite number of recursion steps, each $\nu(v) \circ \nu(u)$ in the basis $\nu(\widehat{\mathcal{F}})$.*

Proof: The correctness of the formulae in Steps 1,2,4 of Algorithm 1 follows from the fact that $\nu\xi = \nu$. As for Step 3, it uses the fact that $\circ : \mathrm{Sh}(V) \otimes \mathrm{Sh}(V) \to \mathrm{Sh}(V)$ is a $\mathrm{Sh}(V)$-module map.

It is now sufficient to show that each of the steps in Algorithm 1 rewrites $\nu(u) \circ \nu(v)$ expressed in the basis $\nu(\widehat{\mathcal{F}})$ provided that we have already rewritten each $\nu(w_1) \circ \nu(w_2)$ with $(u, v) > (w_1, w_2)$ and each $\nu(w_1) \circ \nu(v)$ such that $u = w_1 w_2$ for some $w_2 \in \widehat{\mathcal{F}} \backslash \{e\}$. This trivially holds for Steps 1–2. For Step 3, it follows from Lemma 7 and condition (33). In Step 4, we have by Definition 7 that $wz \in S_{ut}$ and thus $ut \succ wz$, and then $(u, t) > (w, z)$ by condition 3 in Assumption 1. □

Remark 15 Note that the order in which the steps in Algorithm 1 are considered does not affect the proof of Proposition 5, however it does in general change the actual algorithm if the cases in Steps 1,3,4 are not disjoint. □

Remark 16 Assumption 1 implies that (28) and (29) hold. Otherwise, condition 1 in Assumption 1 would not be satisfied. □

If one wants to avoid rational coefficients in the rewriting process, then the $\mathbb{Z}$-basis $\psi(\widehat{\mathcal{F}}) = \{\psi(u) = \nu(u)/\sigma(u): \ u \in \widehat{\mathcal{F}}\}$ can be used instead. Algorithm 1 then leads to the following algorithm, that under Assumption 1, can be used to express each $\psi(v) \circ \psi(u)$ in the basis $\psi(\widehat{\mathcal{F}})$.

Algorithm 2 Given $u, v \in \widehat{\mathcal{F}}\backslash\{e\}$,

1. If $u = w^k$, $v = u^l$, where $k, l \geq 1$ and $w \in \widehat{\mathcal{F}}\backslash\{e\}$, then

$$\psi(u) \circ \psi(v) := k(t^{k-1}, t^l)\, \psi(w^{k+l}),$$

2. Otherwise, if $(u, v) > (v, u)$ then

$$\psi(u) \circ \psi(v) := k(u, v)\, \psi(uv) - \psi(v) \circ \psi(u),$$

3. Otherwise, if $(u, v) \in \mathcal{S}$, then, choose $w_1, w_2 \in \widehat{\mathcal{F}}\backslash\{e\}$ such that (33) holds, and

$$\psi(u) \circ \psi(v) := \frac{1}{k(w_1, w_2)}\, \psi(w_1) \circ (\psi(w_2) \circ \psi(v)),$$

4. Otherwise, $v = t^k$, $k \geq 1$. $t \in \widehat{\mathcal{T}}$ and $\min(u) < t$, and

$$\psi(u) \circ \psi(v) := k(u, t^{k-1})\, r(u, t)\, \psi(w) \circ \psi(z),$$

   where $w \in \widehat{\mathcal{F}}$ and $z \in \widehat{\mathcal{T}}$ are such that $(t^{k-1}v) \circ t = w \circ z = \Gamma(wz)$,

where $k(u, v) = \sigma(uv)/(\sigma(u)\sigma(v)) \in \mathbb{Z}$ and $r(u, t) = \sigma(u \circ t)/(\sigma(u)\sigma(t)) \in \mathbb{Z}$ for each $u, v \in \mathcal{F}$ and $t \in \mathcal{T}$.

Remark 17 In order to completely avoid fractional numbers, in condition 2 of Assumption 1, there must exist $w_1, w_2 \in \widehat{\mathcal{F}}\backslash\{e\}$ satisfying (33) such that w_1 and w_2 have no common factors, so that $k(w_1, w_2) = 1$ in Step 3 of Algorithm 2. In the particular case of the partial order $<$ and the set $\mathcal{S}$ given in Definition 9, this will be accomplished by choosing $w_1 w_2 \in \widehat{\mathcal{F}}\backslash\{e\}$ in Step 3 of Algorithm 2 as $w_1 = t^k$, where $t = \max(w)$ and $k \geq 1$ is such that $t > \max(w_2)$, $w = t^k w_2$. □

5 Lie series and the CBH formula

5.1 The exponential and the logarithm

We next present some known results about arbitrary graded connected commutative Hopf algebras, which will be later applied to the particular cases of $\mathcal{H}_R(V)$ and $\mathrm{Sh}(V)$. Let $\mathcal{H}$ be a commutative graded connected Hopf algebra with unity element $1_{\mathcal{H}}$, coproduct $\Delta_{\mathcal{H}}$, counit $\epsilon_{\mathcal{H}}$, and antipode $S_{\mathcal{H}}$. Let us denote as $\mathcal{H}^+$ the augmentation ideal $\ker \epsilon_{\mathcal{H}}$ of $\mathcal{H}$. Then, as $\mathcal{H}$ is graded connected, $\mathcal{H} = \mathbb{Q}1_{\mathcal{H}} \oplus \mathcal{H}^+$.

Given an arbitrary algebra $\mathcal{A}$ (with multiplication $\mu_{\mathcal{A}}$ and unity map $\eta_{\mathcal{A}} : \mathbb{Q} \to \mathcal{A}$) the coalgebra structure of $\mathcal{H}$ endows the set of linear homomorphisms $\hom(\mathcal{H}, \mathcal{A})$ of $\mathcal{H}$ onto $\mathcal{A}$ with an algebra structure (over $\mathbb{Q}$), with unity element $\eta_{\mathcal{A}}\epsilon_{\mathcal{H}} : \mathcal{H} \to \mathcal{A}$, and multiplication $*$ defined as follows. Given $\alpha, \beta \in \hom(\mathcal{H}, \mathcal{A})$,

$$(\alpha * \beta)(u) = \mu_{\mathcal{A}}(\alpha \otimes \beta)\Delta_{\mathcal{H}}(u), \qquad \text{for each } u \in \mathcal{H}. \tag{34}$$

In particular, when $\mathcal{A} = \mathcal{H}$, the algebra structure on $\hom(\mathcal{H}, \mathcal{H})$ is called the convolution algebra [23] (and $*$ the convolution product). Actually, the antipode $S_{\mathcal{H}}$ is defined as the inverse in the convolution algebra of the identity map $\mathrm{id}_{\mathcal{H}}$ in $\mathcal{H}$.

Definition 10 *Given an algebra $\mathcal{A}$ (over $\mathbb{Q}$). If $\alpha \in \hom(\mathcal{H}, \mathcal{A})$, and $\alpha(1_{\mathcal{H}}) = 1$, then the logarithm of α is a new linear map $\log \alpha \in \hom(\mathcal{H}, \mathcal{A})$ defined as*

$$\log \alpha(1_{\mathcal{H}}) \;=\; 0, \quad \log \alpha(u) = \sum_{k=1}^{|u|} \frac{(-1)^{k+1}}{k}(\alpha - \eta_{\mathcal{A}}\epsilon_{\mathcal{H}})^{*k}(u), \qquad \textit{for each } u \in \mathcal{H}^+. \tag{35}$$

If $\beta \in \hom(\mathcal{H}, \mathcal{A})$, and $\beta(1_{\mathcal{H}}) = 0$, then the exponential of β is a new linear map $\exp \beta \in \hom(\mathcal{H}, \mathcal{A})$ defined as

$$\exp \alpha(1_{\mathcal{H}}) \;=\; 1, \quad \exp \beta(u) = \sum_{k=1}^{|u|} \frac{1}{k!}(\beta)^{*k}(u), \qquad \textit{for each } u \in \mathcal{H}^+. \tag{36}$$

Proposition 6 *Given $\alpha, \beta \in \hom(\mathcal{H}, \mathcal{A})$ with $\alpha(1_{\mathcal{H}}) = 1$ and $\beta(1_{\mathcal{H}}) = 0$, it holds that $\log \exp \beta = \beta$ and $\exp \log \alpha = \alpha$.*

Remark 18 Proposition 6 implies that, as an alternative to (35), $\beta = \log \alpha$ can be determined with the recursion obtained by solving $\beta(u)$ from (36). Another interesting recursion is

$$\beta = \alpha + \sum_{k=1}^{|u|-1} \frac{B_k}{k!}(\beta^{*k} * \alpha), \tag{37}$$

where $\{B_k\}$ is the sequence of Bernoulli numbers, that is, $z/(e^z - 1) = 1 + \sum_{k \geq 1} B_k/k!\, z^k$ (in particular, $B_1 = -1/2$, $B_2 = 1/12$, and $B_{2k+1} = 0$ for $k \geq 1$). □

5.2 Affine group schemes and associated Lie algebras

If $\mathbb{K}$ is a commutative algebra, then $\hom(\mathcal{H},\mathbb{K})$ has a $\mathbb{K}$-algebra structure, and the subspace of $\hom(\mathcal{H},\mathbb{K})$ of algebra homomorphisms forms a group, that we denote as $G_{\mathcal{H}}(\mathbb{K})$. Actually, $G_{\mathcal{H}}$ is an affine group scheme, that is, a functor from commutative algebras to groups. The inverse of $\alpha \in G_{\mathcal{H}}(\mathbb{K})$ can be determined in terms of the antipode S of $\mathcal{H}$ as follows. For each $u \in \mathcal{H}$, $\alpha^{-1}(u) = \alpha(S_{\mathcal{H}}(u))$. The definition (35) of the logarithm can be applied for $\alpha = \mathrm{id}$ (the identity map in $\mathcal{H}$) to give $\log \mathrm{id}_{\mathcal{H}}$. Then, if $\alpha \in G_{\mathcal{H}}(\mathbb{K})$, it holds that $\log\alpha(u) = \alpha(\log \mathrm{id}(u))$ for each $u \in \mathcal{H}$.

A linear map $\beta \in \hom(\mathcal{H},\mathbb{K})$ is a $(\eta_{\mathbb{K}}\epsilon_{\mathcal{H}})$-derivation if $\beta(uv) = \eta_{\mathbb{K}}\epsilon_{\mathcal{H}}(u)\beta(v) + \eta_{\mathbb{K}}\epsilon_{\mathcal{H}}(v)\beta(u)$. It can be seen that, if $\alpha \in G_{\mathcal{H}}(\mathbb{K})$, then $\beta = \log\alpha$ is a $(\eta_{\mathbb{K}}\epsilon_{\mathcal{H}})$-derivation. Conversely, if $\beta \in \hom(\mathcal{H},\mathbb{K})$ is a $(\eta_{\mathbb{K}}\epsilon_{\mathcal{H}})$-derivation, then $\exp(\beta) \in G_{\mathcal{H}}(\mathbb{K})$. We thus denote as $\log(G_{\mathcal{H}}(\mathbb{K}))$ the subspace of $\hom(\mathcal{H},\mathbb{K})$ of $(\eta_{\mathbb{K}}\epsilon_{\mathcal{H}})$-derivations. By definition of $(\eta_{\mathbb{K}}\epsilon_{\mathcal{H}})$-derivation, $\beta \in \log(G_{\mathcal{H}}(\mathbb{K}))$ if and only if $u \in \mathbb{Q}\,1_{\mathcal{H}} \oplus (\mathcal{H}^+)^2 \subset \ker\beta$. It is straightforward to check that $\log(G_{\mathcal{H}}(\mathbb{K}))$ has a Lie algebra structure (over $\mathbb{Q}$, but also over $\mathbb{K}$) under the bracket $[\beta_1,\beta_2] = \beta_1 * \beta_2 - \beta_2 * \beta_1$.

If $\mathcal{H}$ is freely generated as an algebra by a set $\mathcal{T}_{\mathcal{H}} \subset \mathcal{H}$ (such set always exists for commutative graded connected Hopf algebras over $\mathbb{Q}$) then the elements of both $G_{\mathcal{H}}(\mathbb{K})$ and $\log(G_{\mathcal{H}}(\mathbb{K}))$ are determined by its values for $t \in \mathcal{T}_{\mathcal{H}}$.

5.3 The case of the Hopf algebra $\mathcal{H}_R(V)$

Let us now consider the Hopf algebra $\mathcal{H}_R$ of rooted trees decorated by D. In this case, we denote $G_{\mathcal{H}}$ simply as G. In what follows, $\mathbb{K}$ denotes a commutative algebra over $\mathbb{Q}$. Recall that $\mathcal{H}_R$ is freely generated as an algebra by the set $\mathcal{T}$ of decorated rooted trees, and thus, given $\beta \in \log(G(\mathbb{K}))$, $\beta(u) = 0$ for each $u \in \mathcal{F}\backslash\mathcal{T}$. Hence, (2) and (34) imply that, if $\beta \in \log(G(\mathbb{K}))$ and $\gamma \in \hom(\mathcal{H}_R,\mathbb{K})$, then, given $u \in \mathcal{T}$ and a decorated partially ordered set U representing u, it holds that

$$(\beta * \gamma)(u) = \sum_{x\in U} \beta(P^{\{x\}}(U))\gamma(R^{\{x\}}(U)).$$

This implies in particular that if $\beta_1, \beta_2 \in \log(G(\mathbb{K}))$, then, for each $t \in \mathcal{T}$, given a decorated partially ordered set T (with root r) representing t, it holds that

$$[\beta_1,\beta_2](t) = \sum_{x\in T\backslash\{r\}} \left(\beta_1(P^{\{x\}}(T))\beta_2(R^{\{x\}}(T)) - \beta_2(P^{\{x\}}(T))\beta_1(R^{\{x\}}(T))\right). \qquad (38)$$

This formula for the bracket of the Lie algebra associated to the affine group scheme G was first given (for the non-decorated case, i.e. $\#D = 1$) by Dür [7].

Next we obtain explicit formulae for $\exp\beta$ when $\beta \in \log(G(\mathbb{K}))$ (i.e. when $\beta(u) = 0$ if $u \in \mathcal{F}\backslash\mathcal{T}$) and $\log\alpha$ when $\alpha \in G(\mathbb{K})$.

Definition 11 *Given $\beta \in \log(G(\mathbb{K}))$, we define β' as the unique map $\beta' \in G(\mathbb{K})$ such that $\beta'(t) = \beta(t)$ for each $t \in \mathcal{T}$, so that $\beta'(t_1\cdots t_m) = \beta(t_1)\cdots\beta(t_m)$ if $t_1,\ldots,t_m \in \mathcal{T}$.*

From (2) and Definition 10, one directly obtains the following.

Lemma 9 *Given $\beta \in \log(G(\mathbb{K}))$, $t \in \mathcal{T}$, let T be a partially ordered set decorated by D representing t. Then it holds that*

$$\exp \beta(t) = \sum_{Z \in K(T)} \frac{p(Z)}{|Z|!} \beta'(C^Z(T))$$

where $K(T)$ is the familly of decorated partially ordered subsets Z of T with the same root as T (with decoration and partial order inherited from T) and $p(Z)$ is the number of different total orderings of the set Z that preserve the partial ordering in Z.

Lemma 10 *Given $\alpha \in G(\mathbb{K})$, $t \in \widehat{\mathcal{T}}$, let T be a partially ordered set decorated by D representing t. Then it holds that*

$$\log \alpha(t) = \sum_{Z \in K(T)} \omega(Z)\, \alpha(C^Z(T)) \tag{39}$$

where $K(T)$ is given in Lemma 9 and

$$\omega(Z) = \sum_{k \geq 1} \frac{(-1)^{k+1}}{k} \omega^{(k)}(Z),$$

where, for each $k \geq 1$, $\omega^{(k)}(Z)$ is the number of different ordered partitions $(Z_1, \ldots, Z_k)$ of Z satisfying that

$$x \in Z_i, \quad y \in Z_j, \quad x < y \quad \Longrightarrow \quad i < j. \tag{40}$$

Remark 19 Note that both $p(Z)$ and $\omega(Z)$ for decorated partially ordered sets Z in Lemma 9 and Lemma 10 respectively only depend on the structure of rooted tree in Z (both are decoration-blind). This is also the case of the factorial $t!$ of decorated rooted trees given in Definition 1. □

Remark 20 Lemma 9 and Lemma 10 imply the following. Let $\alpha \in G(\mathbb{Q})$ and $\beta \in \log(G(\mathbb{Q}))$ be such that, given $t \in \mathcal{T}$, $\alpha(t) = \beta(t) = 1$ if $|t| = 1$ and $\alpha(t) = \beta(t) = 0$ otherwise. Then, $p(t) = |t|! \exp \alpha(t)$ and $\omega(t) = \log \beta(t)$ for each $t \in \mathcal{T}$. This is true for arbitrary D, and in particular for $\#D = 1$, that is, $\mathcal{T}$ being the set of standard rooted trees. □

Remark 21 It can be shown by combinatorial arguments that $|t|! = p(t)t!$ for each rooted tree t. Actually, Remark 20 can be interpreted using the standard terminology in the theory of numerical integration of ordinary differential equations that $p(t)/|t|!$ is the B-series coefficient (associated to the rooted tree t) of the exact solution of the differential equation, which is known to be $1/t!$, while $\omega(t)$ is the B-series coefficient of the modified equation of the explicit Euler method. □

According to Remark 21, we have the following.

Lemma 11 *Given a forest $u \in \mathcal{F}$, let U be a decorated partially ordered set representing U, and let $p(U)$ be the number of different possible total relations of U that extends its partial ordering, then it holds that $|u|! = u!\,p(U)$.*

Remark 20 together with Lemmas 9–11 imply the following two results.

Proposition 7 *Given $\beta \in \log(G(\mathbb{K}))$, $t \in \mathcal{T}$, let T be a partially ordered set decorated by D representing t. Then it holds that*

$$\exp \beta(t) = \sum_{Z \in K(Z)} \frac{1}{Z!} \beta'(C^Z(T))$$

where $K(Z)$ is given as in Lemma 9.

Proposition 8 *Given $\alpha \in G(\mathbb{K})$, $t \in \widehat{\mathcal{T}}$, let T be a partially ordered set decorated by D representing t. Then (39) holds with $\omega \in \log(G(\mathbb{Q}))$ being uniquely determined by $\exp \omega \in G(\mathbb{Q})$ such that, given $t \in \mathcal{T}$, $\exp \omega(t) = 1$ if $|t| = 1$ and $\exp \omega(t) = 0$ otherwise.*

The coefficients $\omega(t)$ in (8) can recursively be obtained for each (undecorated) rooted tree t as follows. Note that $\omega(t) = 1$ if $|t| = 1$.

Lemma 12 *Let t be a rooted tree of degree $|t| > 1$ and u be the forest obtained by removing the root of t, then it holds that*

$$\omega(t) = \sum_{k=1}^{|t|-1} \frac{B_k}{k!} \omega^{*k}(u). \tag{41}$$

More specifically, let U be a partially ordered set representing the forest of rooted trees u, and let $K(U)$ be the set of partially ordered subsets V of U that include all the roots of U. Then it holds that

$$\omega(t) = \sum_{V \in K(U)} \frac{B_{|V|}}{V!} \omega'(C^V(U)). \tag{42}$$

Proof: Recursion (41) follows from (37) by observing that the following holds. If $\alpha \in G(\mathbb{K})$ is such that, given $t \in \mathcal{T}$, it holds that $\alpha(t) = 1$ provided that $|t| = 1$ and $\alpha(t) = 0$ otherwise, then $(\gamma * \alpha)(t) = \gamma(u)$ for arbitrary $\gamma \in \hom(\mathcal{H}_R, \mathbb{K})$, $t = B_d(u) \in \mathcal{T}$. Successive application of (2) applied to (41) gives (42) with $1/V!$ replaced by $p(V)/|t|!$, so that Lemma 11 finally leads to (42). □

5.4 Lie series

Let us now consider $\mathcal{H} = \mathrm{Sh}(V)$, and denote $G_{\mathcal{H}}$ as $\widehat{G}$. Note that in the particular case of $\mathbb{K} = \mathbb{Q}$, we have that $\hom(\mathrm{Sh}(V), \mathbb{Q}) = \mathrm{Sh}(V)^*$, and that when $\alpha, \beta \in \mathrm{Sh}(V)^*$, then $\alpha * \beta$ coincides with the product $\alpha\beta$ given in (22).

Given a commutative algebra $\mathbb{K}$, the $\mathbb{K}$-algebra $\hom(\mathrm{Sh}(V), \mathbb{K})$ (with product $*$) is isomorphic (using the terminology in [20]) to the $\mathbb{K}$-algebra of formal series $\mathbb{K}\langle\langle D\rangle\rangle$ of words over the alphabet D (with concatenation product $\top$), each $\widehat{\alpha} \in \hom(\mathrm{Sh}(V), \mathbb{K})$ being identified with the formal series $\sum_{w\in\mathcal{W}} \widehat{\alpha}(w)\, w$, where $\mathcal{W}$ denotes the set of words on the alphabet D (including the empty word $\widehat{e}$). Furthermore, the Lie algebra $\log(\widehat{G}(\mathbb{K}))$ over $\mathbb{K}$ is isomorphic to the Lie algebra (over $\mathbb{K}$) of Lie series over the alphabet D with coefficients in $\mathbb{K}$ (characterization (iv) of Lie series in Theorem 3.1 of [20] says that $\widehat{\alpha} \in \hom(\mathrm{Sh}(V), \mathbb{K})$ is a Lie series if and only if $\widehat{\alpha}$ is a $(\eta_{\mathbb{K}}\widehat{\epsilon})$-derivation). This implies that $\widehat{\alpha} \in \hom(\mathrm{Sh}(V), \mathbb{K})$ is the exponential of a Lie series if and only if $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$.

Consider for each $u \in \widehat{\mathcal{F}}$ a $\mathbb{Z}$-linear combination of words P_u defined recursively as follows.

Definition 12 *For each $d \in D$, $P_d = d$, $P_{\widehat{e}} = \widehat{e}$, for each Hall rooted trees $t \in \widehat{\mathcal{T}}$ of degree $|t| > 1$, $P_t = P_{t''} \top P_{t'} - P_{t'} \top P_{t''}$, where (t', t'') is the standard decomposition of t, and for each $u = t_1 \cdots t_m$ where $t_1, \ldots, t_m \in \widehat{\mathcal{T}}$, $m \geq 1$, $t_1 \geq \cdots \geq t_m$, $P_u = P_{t_1} \top \cdots \top P_{t_m}$.*

Thus [20], $\{P_t : \ t \in \widehat{\mathcal{T}}\}$ is a Hall basis of the free Lie $\mathbb{K}$-algebra $\mathcal{L}_{\mathbb{K}}(D)$ over the alphabet D, and $\{P_u : \ u \in \widehat{\mathcal{F}}\}$ the Poincaré-Witt-Birkhoff basis of $\mathbb{K}\langle D\rangle$ corresponding to the Hall basis $\{P_t : \ t \in \widehat{\mathcal{T}}\}$ of $\mathcal{L}_{\mathbb{K}}(D)$, and according to Definition 5 and Theorem 3, the isomorphism of $\hom(\mathrm{Sh}(V), \mathbb{K})$ and $\mathbb{K}\langle\langle D\rangle\rangle$ identifies each F_u ($u \in \widehat{\mathcal{F}}$) with P_u. Then, for each $\alpha \in \hom(\mathrm{Sh}(V), \mathbb{K})$, the corresponding formal series can be rewritten in terms of that Poincaré-Witt-Birkhoff basis of $\mathbb{K}\langle D\rangle$ as

$$\sum_{w\in\mathcal{W}} \widehat{\alpha}(w)\, w = \sum_{u\in\widehat{\mathcal{F}}} \frac{\widehat{\alpha}(\nu(u))}{\sigma(u)}\, P_u$$

We then have that, given $\widehat{\alpha}, \widehat{\beta} \in \hom(\mathrm{Sh}(V), \mathbb{K})$,

$$\left(\sum_{u\in\widehat{\mathcal{F}}} \frac{\widehat{\alpha}(\nu(u))}{\sigma(u)}\, P_u\right) \top \left(\sum_{u\in\widehat{\mathcal{F}}} \frac{\widehat{\beta}(\nu(u))}{\sigma(u)}\, P_u\right) = \sum_{u\in\widehat{\mathcal{F}}} \frac{(\widehat{\alpha} * \widehat{\beta})(\nu(u))}{\sigma(u)}\, P_u,$$

and thus, in order to compute the product of two such series in terms of the PWB basis $\{P_u : \ u \in \widehat{\mathcal{F}}\}$ (that is, in terms of the coefficients $\widehat{\alpha}(\nu(u)), \widehat{\beta}(\nu(u))$, $u \in \widehat{\mathcal{F}}$), it is only required to have the coproduct $\widehat{\Delta}\nu(u)$, $u \in \widehat{\mathcal{F}}$, written in terms of this basis, which can be obtained efficiently by means of recursion (13) and Algorithm 1.

It is often required in applications to obtain, given $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$, the Lie series $\widehat{\beta} = \log \widehat{\alpha}$. In order to express such Lie series in terms of a basis associated to a Hall set (i.e a Hall set

$\widehat{\mathcal{T}}$ of decorated rooted trees), we need to compute the coefficients $\log\alpha(\nu(t))/\sigma(t)$ of the term of the Hall basis associated to each $t \in \widehat{\mathcal{T}}$. In order to do this, we need to be able to perform the product (34) in $\mathrm{hom}(\mathrm{Sh}(V), \mathbb{K})$ (for instance, as we have just mentioned, by means of recursion (13) and Algorithm 1). Once the product $*$ is implemented, the required values $\widehat{\beta}(\nu(t)) = \log\alpha(\nu(t))$ can be obtained either by applying the definition in power series (35) of the logarithm, or, for instance, by means of some recursion based on the fact that the logarithm is the inverse of the exponential (36), for instance (37).

Consider an arbitrary algebra $\mathcal{A}$ over $\mathbb{Q}$. For each $\widehat{\alpha}, \widehat{\beta} \in \mathrm{hom}(\mathrm{Sh}(V), \mathcal{A})$, we obviously have that $\alpha, \beta \in \mathrm{hom}(\mathcal{H}, \mathcal{A})$ for $\alpha = \widehat{\alpha}\nu$ and $\beta = \widehat{\beta}\nu$. Then, (19) implies that

$$(\widehat{\alpha} * \widehat{\beta})\nu \;=\; \alpha * \beta, \quad [\widehat{\alpha}, \widehat{\beta}]\nu \;=\; [\alpha, \beta], \tag{43}$$

$$(\log\widehat{\alpha})\nu \;=\; \log\alpha, \quad (\exp\widehat{\beta})\nu \;=\; \exp\beta. \tag{44}$$

In addition, given a commutative algebra $\mathbb{K}$, it holds that $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$ (resp. $\widehat{\beta} \in \log(\widehat{G}(\mathbb{K}))$) if and only if $\alpha = \widehat{\alpha}\nu \in G(\mathbb{K})$ (resp. $\beta = \widehat{\beta}\nu \in \log(G(\mathbb{K}))$). We thus can apply the results on $\mathcal{H}_R$, and in particular, those in Subsection 5.3, to work in the algebra $\mathrm{hom}(\mathrm{Sh}(V), \mathcal{A})$, the Lie algebra $\log(\widehat{G}(\mathbb{K}))$ of Lie series, and the group $\widehat{G}(\mathbb{K})$ of exponentials of Lie series. Thus, if the values of $\alpha = \widehat{\alpha}\nu \in G(\mathbb{K})$ for arbitrary decorated rooted trees in $\mathcal{T}$ are available then the coefficients $\log\widehat{\alpha}(\nu(t))$ $(t \in \widehat{\mathcal{T}})$ of the Lie series $\log\widehat{\alpha}$ of an arbitrary $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$ can be explicitly obtained by applying Proposition 8 for $\alpha = \widehat{\alpha}\nu$.

In particular, we will explicitly obtain the formal expansion of $\log(\exp(X)\exp(Y))$ as a Lie series over the alphabet $\{X, Y\}$ (known as Hausdorff series, and also as the Campbell-Baker-Hausdorff formula) expressed in an arbitrary Hall basis of the free Lie algebra over $\{X, Y\}$.

5.5 The CBH formula and some generalizations

Let $\widehat{\mathcal{T}}$ be a Hall set of rooted trees decorated by $D = \{x, y\}$, and $\widehat{\mathcal{F}}$ the corresponding set of Hall forests. Consider $P_t \in \log(\widehat{G}(\mathbb{K}))$ $(t \in \widehat{\mathcal{T}})$ given in Definition 12, and identify the symbols X and Y with P_x and P_y respectively. The CBH formula then reads

$$\log(\exp(X)\exp(Y)) = \sum_{t \in \widehat{\mathcal{T}}} \frac{\beta(t)}{\sigma(t)} P_t, \tag{45}$$

where for each $t \in \widehat{\mathcal{T}}$, $\beta(t) = \widehat{\beta}(\nu(t))$, $\widehat{\beta} = \log\widehat{\alpha}$, $\widehat{\alpha} = \exp(\widehat{\beta}_x) * \exp(\widehat{\beta}_y) \in \widehat{G}(\mathbb{Q})$, and $\widehat{\beta}_d \in \log(\widehat{G}(\mathbb{K}))$ for $d = x, y \in D$ are determined by $\widehat{\beta}_d(d) = 1$ and $\widehat{\beta}_d(w) = 0$ for any word $w \neq d$ (note that each $\widehat{\beta}_d$ coincides with F_d given in Definition 5). Alternatively, we have by virtue of (43)–(44) that $\beta = \log\alpha$, where $\alpha = \widehat{\alpha}\nu = \exp(\beta_x) * \exp(\beta_y) \in G(\mathbb{Q})$, and $\beta_d = \widehat{\beta}_d\nu \in \log(G(\mathbb{Q}))$ for each $d \in D = \{x, y\}$. That is, given $u \in \mathcal{F}$, $\beta_d(u) = 1$ if $u = d$ and $\beta_d = 0$ otherwise. The following result explicitly gives the coefficients $\beta(t)$ in the CBH formula (45).

Proposition 9 *Consider $D = \{x, y\}$ and $\beta_d \in \log(G(\mathbb{K}))$ defined for each $d \in D$ as follows. Given $u \in \mathcal{F}$, $\beta_d(u) = 1$ if $u = d$ and $\beta_d = 0$ otherwise. Let $\alpha = \exp(\beta_x) * \exp(\beta_y)$ and $\beta = \log \alpha$. Given $t \in \mathcal{T}(D)$, let T be a decorated partially ordered set representing t, then*

1. *$\alpha(t) = 1/C^V(T)!$ if there exists a subset V of T satisfying (3) such that all the vertices of $P^V(T)$ are decorated by x and all the vertices of $R^V(T)$ are decorated by y (there is at most one such subset V) and $\alpha(t) = 0$ otherwise.*

2. *and $\beta(t)$ is given in terms of α by Proposition 8, or directly as*

$$\beta(t) = \sum_{Z \in M(T)} \frac{\omega_{x,y}(Z)}{C^Z(T)!}$$

where $M(t)$ is the set of decorated partially ordered subsets Z of T with the same root as T such that each decorated rooted tree in the forest $C^Z(T)$ is decorated either only by x or only by y, and $\omega_{x,y}(z) \in \mathbb{Q}$ is given for each $z \in \mathcal{T}$ as follows. Let Z be a decorated partially ordered set representing z, then

$$\omega_{x,y}(Z) = \sum_{Z^* \in N(Z)} \omega(Z^*)$$

where $N(Z)$ is the set of decorated partially ordered subsets of Z with the same root as Z and the same number of vertices decorated by y as Z.

Proof: Proposition 8 implies that $\exp \beta_d(t) = 1/t!$ if all the vertices in t are decorated by d and $\exp \beta_d(t) = 0$ otherwise. As for $\alpha = \exp(\beta_x) * \exp(\beta_y) \in G(\mathbb{Q})$, (34) and (2) lead to first statement of Proposition 9. Application of Proposition 8 to such $\alpha \in G(\mathbb{Q})$ leads to the required result, by observing that, if $Z \in M(T)$, then $N(Z)$ coincides with the set of decorated partially ordered subsets Z^* of Z such that $\alpha(C^{Z^*}(T)) = C^Z(T)!$. □

Remark 22 It is not difficult to generalize Proposition 9 to obtain similar explicit formulae for the coefficients of the Lie series expansion of $\log(\exp(X_1) \cdots \exp(X_m))$ for the symbols X_i. □

Remark 23 As mentioned in Remark 8, for each $t \in \widehat{\mathcal{T}}$, there exists a decorated rooted tree $t^* \in \mathcal{T}$ such that $\nu(t^*) = \nu(t)/\sigma(t)$, so that $\beta(t)/\sigma(t) = \widehat{\beta}(\nu(t))/\sigma(t)$ can be replaced in the CBH formula (45) by $\beta(t^*)$ as given by Proposition 9 for the decorated rooted tree t^*. □

Remark 24 In practice, if the coefficients $\beta(t) = \widehat{\beta}(\nu(t))$ in (45) for Hall rooted trees up to a certain degree are required, they can be more efficiently computed following different recursive procedures, for instance, based on (37). From a computational point of view, it may be preferable to use algorithms that only involve the sets of Hall rooted trees $\widehat{\mathcal{T}}$ and

Hall forests $\widehat{\mathcal{F}}$, as the numbers of decorated rooted trees of a given degree increase very fast compared to Hall rooted trees.

The task of obtaining $\widehat{\beta}(\nu(t))$ for $t \in \widehat{\mathcal{T}}$ is simplified if the Hall set of rooted trees $\widehat{\mathcal{T}}$ is constructed in such a way that $x > y$. In that case, it holds for $\widehat{\alpha} = \exp(\widehat{\beta}_x) * \exp(\widehat{\beta}_y)$ that $\widehat{\alpha}(\nu(t)) = 1$ if $t = x$ or $t = y$, and $\widehat{\alpha}(\nu(t)) = 0$ otherwise. It then remains to obtain the values of $\widehat{\beta} = \log \widehat{\alpha}$ for $\nu(t)$, $t \in \widehat{\mathcal{T}}$, which can be done efficiently, as indicated in Subsection 5.4, with the help of (13) and Algorithm 1. □

Remark 25 The CBH formula can also be recursively obtained working exclusively in the free Lie algebra generated by the symbols $\{X, Y\}$, which involves Bernoulli numbers [24] as in (37). The resulting recursion does not seem however to be advantageous in our framework. □

Further generalizations of the CBH formula can be obtained with the help of recursion (13) and Algorithm 1. Given Lie series $\widehat{\beta}_1, \ldots, \widehat{\beta}_m$ over an alphabet D with a commutative $\mathbb{Q}$-algebra $\mathbb{K}$ as base ring (we can interpret them, using our notation, as elements in $\log(\widehat{G}(\mathbb{K}))$), a new Lie series of the form

$$\widehat{\beta} := \log(\exp(\widehat{\beta}_1) * \cdots * \exp(\widehat{\beta}_m))$$

can be similarly expressed in a Hall basis of $\mathcal{L}(D)$, with (13) and Algorithm 1 as the main tools to obtain the coefficients $\widehat{\beta}(\nu(t))/\sigma(t)$ corresponding to the element P_t ($t \in \widehat{\mathcal{T}}$) of the Hall basis of $\mathcal{L}(D)$. This is useful, for instance, in the context of numerical integration of ordinary differential equations, in particular, when studying composition integrators [15, 16]. Note that, according to (43)–(44), the coefficients $\widehat{\beta}(\nu(t))$ ($t \in \widehat{\mathcal{T}}$) of the Lie series $\widehat{\beta}$ can alternatively be obtained as $\beta(t)$, where $\beta = \log(\exp(\beta_1) * \cdots * \exp(\beta_m))$ and $\beta_i = \widehat{\beta}_i \nu$ belong to $\log(G(\mathbb{K}))$, and thus the computations can be performed with the tools developed in Subsection 5.3.

5.6 Continuous CBH formulae

A continuous version of CBH formula was first considered in [5], and since then it has been considered in the literature in several contexts. For instance, in nonlinear control theory (see [11, 12, 21] and references therein), stochastic differential equations [2], and in Lie group techniques of numerical integration of ordinary differential equations [10]. The problem of expressing the continuous CBH formula in a basis of $\mathcal{L}(D)$ can be reduced to writing in terms of this basis the Lie series (with coefficients in a commutative $\mathbb{Q}$-algebra) obtained as the logarithm $\log \widehat{\alpha}$ of a particular $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$ representing a series of iterated integrals. In nonlinear control theory, $\mathbb{K}$ is the vector space of Riemann-integrable real-valued functions, and $\widehat{\alpha}$ represents the so-called Chen-Fliess series. In stochastic differential equations, $\mathbb{K}$ is the algebra of (real-valued) stochastic processes, and the integral operators correspond to the Stratonovich integral formulation of stochastic differential equations [2]. In Lie group integrators [10], the continuous CBH formula arises, for instance, when the study of numerical methods for matrix differential equations of the form $X' = B(t)X$ requires rewriting its solution as $X(t) = \exp(\sum_{k\geq 1} Y_k t^k)$ provided that $B(t) = \sum_{k\geq 0} B_k t^k$.

The problem can be stated in algebraic terms as follows. Consider a commutative algebra $\mathbb{K}$ over $\mathbb{Q}$ and a $\mathbb{Q}$-linear map $\int : \mathbb{K} \to \mathbb{K}$ such that the following property (integration by parts) holds,

$$(\int \lambda)(\int \mu) = \int(\lambda \int \mu) + \int(\mu \int \lambda), \quad \text{for each} \quad \lambda, \mu \in \mathbb{K}. \tag{46}$$

Let $\mathcal{A}$ be a $\mathbb{K}$-algebra, and let $\int_{\mathcal{A}} : \mathcal{A} \to \mathcal{A}$ be a $\mathbb{Q}$-linear map such that $\int_{\mathcal{A}} \eta_{\mathcal{A}} = \eta_{\mathcal{A}} \int$ for the unity map $\eta_{\mathcal{A}} : \mathbb{K} \to \mathcal{A}$ in the $\mathbb{K}$-algebra $\mathcal{A}$. With some abuse of notation, we will write the map $\int_{\mathcal{A}}$ also as $\int$. Assume that, given $b \in \mathcal{A}$, the equation

$$a = 1_{\mathcal{A}} + \int(ab) \tag{47}$$

has a unique solution. Fixed point iteration gives the formal solution

$$a = 1_{\mathcal{A}} + \int b + \int(\int b)b + \int(\int(\int b)b)b + \cdots \tag{48}$$

Let us denote as $\mathcal{A}_{\text{cons}}$ the subalgebra of $\mathcal{A}$ defined by

$$\mathcal{A}_{\text{cons}} = \{a \in \mathcal{A} : \int(ba) = (\int b)a, \text{ for each } b \in \mathcal{A}\},$$

and similarly for $\mathbb{K}_{\text{cons}}$. Assume that, in (47), $b = \sum_{d\in D} \lambda_d \, a_d$ where D is a set of indices, and for each $d \in D$, $\lambda_d \in \mathbb{K}$ and $a_d \in \mathcal{A}_{\text{cons}}$. In that case, (49) can be rewritten as

$$a = 1_{\mathcal{A}} + \textstyle\sum_{d\in D}(\int \lambda_d)a_d + \sum_{d_1,d_2\in D}(\int(\int \lambda_{d_1})\lambda_{d_2})a_{d_1}a_{d_2} + \cdots$$

or equivalently,

$$a = \sum_{w\in\mathcal{W}} \widehat{\alpha}(w)\, a_w, \tag{49}$$

where $\mathcal{W}$ denotes the set of words on the alphabet D (including the empty word $\widehat{e}$), and $\widehat{\alpha}(w) \in \mathbb{K}$ and $a_w \in \mathcal{A}_{\text{cons}}$ are recursively defined as follows.

$$a_{\widehat{e}} = 1_{\mathcal{A}}, \qquad a_{w\top d} = a_w a_d, \quad w \in \mathcal{W}, \quad \text{for each} \quad d \in D, \tag{50}$$

$$\widehat{\alpha}(\widehat{e}) = 1_{\mathbb{K}}, \qquad \widehat{\alpha}(w\top d) = \int(\widehat{\alpha}(w)\lambda_d), \quad \text{for each} \quad w \in \mathcal{W}, \quad d \in D, \tag{51}$$

Obviously, (51) determines a unique $\widehat{\alpha} \in \hom(\text{Sh}(V), \mathbb{K})$, which turns out to be an algebra map, that is, $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$. To see this, consider for each $d \in D$ the $\mathbb{Q}$-linear map

$$L_d : \mathbb{K} \to \mathbb{K}, \quad L_d(\mu) = \int(\mu\lambda_d), \quad \text{for each} \quad \mu \in \mathbb{K}, \tag{52}$$

and observe that (46) implies that the assumptions of Proposition 2 hold for $\mathcal{A} := \mathbb{K}$ and L_d given for each $d \in D$ in (52), so that there exists a unique algebra map $\widehat{\phi} : \text{Sh}(V) \to \mathbb{K}$ such that $\widehat{\phi} C_d = L_d \widehat{\phi}$, i.e. $\widehat{\phi}(w\top d) = \int(\widehat{\alpha}(w)\lambda_d)$ for each $d \in D$ and $w \in \mathcal{W}$. Hence $\widehat{\phi} = \widehat{\alpha}$.

The map $w \in \mathcal{W} \to a_w \in \mathcal{A}_{\text{cons}}$ extended by linearity to $w \in \text{Sh}(V) \to a_w \in \mathcal{A}_{\text{cons}}$ is actually the unique algebra homomorphism of the algebra $\mathbb{K}\langle D\rangle$ (with concatenation product $\top$) onto the subalgebra of $\mathcal{A}_{\text{cons}} \subset \mathcal{A}$ generated by $\{a_d : \ d \in D\}$, which gives rise to an homomorphism of the algebra of formal series $\mathbb{K}\langle\langle D\rangle\rangle$ (isomorphic to $\hom(\text{Sh}(V), \mathbb{K})$) onto the algebra of series of the form (49)–(50). This shows in particular the following. Given a Hall set $\widehat{\mathcal{T}}$ of rooted trees generated by D and the corresponding set $\widehat{\mathcal{F}}$ of Hall forests, let us denote with some abuse of notation $a_u := a_{P_u}$ for each $u \in \widehat{\mathcal{F}}$. Then it formally holds that for any $\widehat{\alpha} \in \hom(\text{Sh}(V), \mathbb{K})$,

$$\sum_{w\in\mathcal{W}} \widehat{\alpha}(w)\, a_w = \sum_{u\in\widehat{\mathcal{F}}} \frac{\widehat{\alpha}(\nu(u))}{\sigma(u)}\, a_u$$

As a consequence of previous considerations, we have that the formal solution (49) of (47) can be expressed in the form

$$a = \exp\left(\sum_{t\in\widehat{\mathcal{T}}} \frac{\log\widehat{\alpha}(\nu(t))}{\sigma(t)}\, a_t\right). \tag{53}$$

The formal representation (53) of the solution of (47) can be considered as a continuous version of the CBH formula, which can be applied in different contexts, in particular, in those mentioned at the beginning of the present subsection. The practical problem of finding the continuous CBH formula then reduces to obtaining the coefficients $\log\widehat{\alpha}(\nu(t))/\sigma(t)$ for each $t \in \widehat{\mathcal{T}}$. This can be done in terms of Hall rooted trees and forests, as indicated in Subsection 5.4, with the help of (13), Algorithm 1, and either (35) or recursion (37). Alternatively, an explicit formula for $\log\widehat{\alpha}(\nu(t))$ can be obtained by applying Proposition 8 as follows.

Consider the algebra map $\alpha = \widehat{\alpha}\nu \in G(\mathbb{K})$, so that, according to (44), $\log\alpha = (\log\widehat{\alpha})\nu$. Moreover, Theorem 1 and (51) imply that $\alpha B_d = L_d\alpha$ for each $d \in D$, where the $\mathbb{Q}$-linear map $L_d : \mathbb{K} \to \mathbb{K}$ is given in (52). Thus, α is the unique algebra map $\mathcal{H}_R \to \mathbb{K}$ given by Proposition 1 for $\mathcal{A} := \mathbb{K}$ and L_d given by (52). In other words, $\alpha \in G(\mathbb{K})$ can be determined as the unique $\mathbb{Q}$-linear map such that, given $d \in D$, $u \in \mathcal{F}$, $t_1, \ldots, t_m \in \mathcal{T}$,

$$\alpha(e) = 1, \quad \alpha(B_d(u)) = \textstyle\int(\alpha(u)\lambda_d), \quad \alpha(t_1\cdots t_m) = \alpha(t_1)\cdots\alpha(t_m). \tag{54}$$

Recursion (54) thus assigns an iterated integral to each decorated rooted tree and forest. Thus, application of Proposition 8 to $\alpha \in G(\mathbb{K})$ given by (54) provides and explicit formula for the coefficients $\log\alpha(t) = \log\widehat{\alpha}(\nu(t))$, $t \in \widehat{\mathcal{T}}$ in (53).

In [14], iterated integrals are associated to decorated rooted trees as in (54) in the context of renormalization in quantum field theory (there, only finite-type integrals satisfy the integration by parts property (46) that guarantees the existence of $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$ such that $\alpha = \widehat{\alpha}\nu$ for $\alpha \in G(\mathbb{K})$ given in (54)).

It may be of interest to note that a recursion for the coefficients $\beta(t) = \widehat{\beta}(\nu(t))$ for $\widehat{\beta} = \log\widehat{\alpha}$ in the continuous CBH formula (53) that only involves operations in the Lie algebra $\log(\widehat{G}(\mathbb{K}))$ (or $\log(G(\mathbb{K}))$ for that matter) can be obtained, derived from the so-called Magnus expansion (see for instance [10] for a presentation of Magnus formula in the context of Lie group integrators), which can be generalized in our framework provided that the identity

$$(\int a)(\int b) = \int(a \int b) + \int((\int a)b), \quad \text{for each} \quad a, b \in \mathcal{A},$$

holds.

Equation (47) can be generalized by considering formal series expansions of the solution $c \in \mathcal{A}$ of $c = c_0 + \int(cb)$, for prescribed $c_0, b \in \mathcal{A}$. If c_0, b admit expansions of the form $c_0 = \sum_{w \in \mathcal{W}} \widehat{\gamma}_0(w)\, a_w$, $b = \sum_{w \in \mathcal{W}} \widehat{\beta}(w)\, a_w$ with $\alpha_0, \widehat{\beta} \in \hom(\mathrm{Sh}(V), \mathbb{K})$, then $c = \sum_{w \in \mathcal{W}} \widehat{\gamma}(w)\, a_w$, where $\widehat{\gamma} \in \hom(\mathrm{Sh}(V), \mathbb{K})$ is the solution of $\widehat{\gamma} = \widehat{\gamma}_0 + \int(\widehat{\gamma} * \widehat{\beta})$. Alternatively, $c = \sum_{u \in \widehat{\mathcal{F}}} \frac{\gamma(u)}{\sigma(u)} a_u$, where $\beta = \widehat{\beta}\nu$, $\gamma_0 = \widehat{\gamma}_0\nu$ and $\gamma \in \hom(\mathcal{H}_R(V), \mathbb{K})$ is the solution of $\gamma = \gamma_0 + \int(\gamma * \beta)$. We thus simply can assume that $\mathcal{A} = \hom(\mathrm{Sh}(V), \mathbb{K})$ or $\mathcal{A} = \hom(\mathcal{H}_R(V), \mathbb{K})$, with $\int_{\mathcal{A}} : \mathcal{A} \to \mathcal{A}$ representing composition with $\int : \mathbb{K} \to \mathbb{K}$, and $\mathcal{A}_{\mathrm{cons}}$ consisting of maps with values in $\mathbb{K}_{\mathrm{cons}}$. In particular, we have that (51) (resp. (54)) is the solution of $\widehat{\alpha} = \eta_{\mathbb{K}}\widehat{\epsilon} + \int(\widehat{\alpha} * \widehat{\beta})$ (resp. $\alpha = \eta_{\mathbb{K}}\epsilon + \int(\alpha * \beta)$). We will proceed with $\mathcal{A} = \hom(\mathrm{Sh}(V), \mathbb{K})$, but similar arguments can be applied for $\mathcal{A} = \hom(\mathcal{H}_R(V), \mathbb{K})$.

If $\widehat{\gamma}_0 \in \mathcal{A}_{\mathrm{cons}}$, then $\widehat{\gamma} = \widehat{\gamma}_0 * \widehat{\alpha}$, with $\widehat{\alpha} \in \mathcal{A}$ being the solution of $\widehat{\alpha} = \eta_{\mathbb{K}}\widehat{\epsilon} + \int(\widehat{\alpha} * \widehat{\beta})$. This is closely related to Chen's convolution formula for the iterated integrals of paths [5]. We have previously shown that, if $\widehat{\beta}(w) = 0$ when $|w| \neq 1$ and $\widehat{\beta}(d) = \lambda_d$ ($d \in D$), then $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$ (actually, it can be shown that $\widehat{\alpha} \in \widehat{G}(\mathbb{K})$ provided that $\widehat{\beta} \in \log(\widehat{G}(\mathbb{K}))$), and thus, in such case, $\widehat{\gamma} \in \widehat{G}(\mathbb{K})$ provided that $\widehat{\gamma}_0 \in \widehat{G}(\mathbb{K})$.

By considering $\mathcal{A} = \hom(\mathcal{H}_R(V), \mathbb{K})$ instead, similar arguments (now with $\int$ not necessarily satisfying (46)) show that, if $\gamma_0 \in \mathcal{A}_{\mathrm{cons}}$, and $\alpha \in \mathcal{A}$ is the solution of $\alpha = \eta_{\mathbb{K}}\epsilon + \int(\alpha * \beta)$ then the solution of $\gamma = \gamma_0 + \int(\gamma * \beta)$ is $\gamma = \gamma_0 * \alpha$, and that $\alpha, \gamma \in G(\mathbb{K})$ provided that $\beta \in \log(G(\mathbb{K}))$ and $\gamma_0 \in G(\mathbb{K})$. This corresponds to Kreimer's generalization [14] of Chen's convolution formula for iterated integrals associated to decorated rooted trees.

In connection with continuous CBH formulae in [11, 21], the following observations may be of interest. Let us denote as $\mathcal{M}$ the image of $\int : \mathbb{K} \to \mathbb{K}$, and assume that there exists a linear map $D : \mathcal{M} \to \mathbb{K}$ that is left inverse of $\int$, so that $D \int \lambda = \lambda$ for each $\lambda \in \mathbb{K}$. In that case, (46) implies that D is a derivation from $\mathcal{M}$ to $\mathbb{K}$, and that $\lambda \circ \mu := \int(\lambda(D\mu))$ for $\lambda \in \mathbb{K}$, $\mu \in \mathcal{M}$ gives a left $\mathbb{K}$-module structure to $\mathcal{M}$ which satisfies (10). This implies that the vector space $\mathcal{M}$ together with the bilinear binary operation $\circ$ has a non-associative algebra structure referred as chronological algebra in [11] and as Zienbel algebra in [21].

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