

# ROOTED TREES, NON-ROOTED TREES AND HAMILTONIAN B-SERIES

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**ABSTRACT.** We explore the relationship between (non-planar) rooted trees and free trees, i.e. without root. We give in particular, for non-rooted trees, a substitute for the Lie bracket given by the antisymmetrization of the pre-Lie product.

**Keywords:** Rooted trees; B-series; Trees; Hamiltonian vector fields.

**Math. subject classification:** 16W30; 05C05; 16W25; 17D25; 37C10

## 1. INTRODUCTION

A striking link between rooted trees and vector fields on an affine space  $\mathbb{R}^n$  has been established by A. Cayley [8] as early as 1857. The interest for this correspondence has been renewed since J. Butcher showed the key role of rooted trees for understanding Runge-Kutta methods in numerical approximation [5, 4, 16]. The modern approach to this correspondence can be summarized as follows: the product on vector fields on  $\mathbb{R}^n$  defined by:

$$(1) \quad \left( \sum_{i=1}^n f_i \partial_i \right) \triangleright \left( \sum_{i=1}^n g_j \partial_j \right) := \sum_{j=1}^n \left( \sum_{i=1}^n f_i (\partial_i g_j) \right) \partial_j$$

is left pre-Lie, which means that for any vector fields  $a, b, c$  the associator  $a \triangleright (b \triangleright c) - (a \triangleright b) \triangleright c$  is symmetric with respect to  $a$  and  $b$ . On the other hand, the free pre-Lie algebra with one generator (on some base field  $k$ ) is the vector space  $\mathcal{T}$  spanned by the planar rooted trees [10, 15]. The generator is the one-vertex tree  $\bullet$ , and the pre-Lie product on rooted trees is given by grafting:

$$(2) \quad s \rightarrow t = \sum_{v \in V(t)} s \rightarrow_v t,$$

where  $s \rightarrow_v t$  is the rooted tree obtained by grafting the rooted tree  $s$  on the vertex  $v$  of the tree  $t$ . Hence for any vector field  $a$  on  $\mathbb{R}^n$  there exists a unique pre-Lie algebra morphism  $\mathcal{F}_a$  from  $\mathcal{T}$  to vector fields such that  $\mathcal{F}_a(\bullet) = a$ . This can be generalized to an arbitrary number of generators, since the free pre-Lie algebra on a set  $D$  of generators is the span of rooted trees with vertices coloured by  $D$ . In this case, for any collection  $\underline{a} = (a_d)_{d \in D}$  of vector fields, there exists a unique pre-Lie algebra morphism  $\mathcal{F}_{\underline{a}}$  from the linear span  $\mathcal{T}_D$  of coloured trees to vector fields on  $\mathbb{R}^n$ , such that  $\mathcal{F}_{\underline{a}}(\bullet_d) = a_d$  for any  $d \in D$ .

The vector fields  $\mathcal{F}_a(t)$  (or  $\mathcal{F}_{\underline{a}}(t)$  in the coloured case) are the *elementary differentials*, building blocks of the B-series [16] which are defined as follows: for any linear form  $\alpha$  on  $\mathcal{T}_D \oplus \mathbb{R}\mathbf{1}$  where  $\mathbf{1}$  is the empty tree, for any collection of vector fields  $\underline{a}$  and for any initial point  $y_0 \in \mathbb{R}^n$ , the corresponding B-series<sup>1</sup> is a formal series in the indeterminate  $h$  given by:

$$(3) \quad B_{\underline{a}}(\alpha, y_0) = \alpha(\mathbf{1})y_0 + \sum_{t \in \mathcal{T}_D} h^{|t|} \frac{\alpha(t)}{\text{sym}(t)} \mathcal{F}_{\underline{a}}(t)(y_0).$$

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<sup>1</sup>Such coloured B-series are sometimes called NB-series in the literature.

Here  $|t|$  is the number of vertices of  $t$ , and  $\text{sym}(t)$  is its symmetry factor, i.e. the cardinal of its automorphism group  $\text{Aut } t$ . For any vector field  $a$ , the exact solution of the differential equation:

$$(4) \quad \dot{y}(t) = a(y(t))$$

with initial condition  $y(0) = y_0$  admits a (one-coloured) B-series expansion at time  $t = h$ , and its approximation by any Runge-Kutta method as well [5, 6, 16]. The formal transformation  $y_0 \mapsto B_a(\alpha, y_0)$  is a formal series with coefficients in  $C^\infty(\mathbb{R}^n, \mathbb{R}^n)$ .

We will be interested in *canonical B-series* [7], i.e. such that the formal transformation  $B_{\underline{a}}(\alpha, -)$  is a symplectomorphism for any collection of hamiltonian vector fields  $\underline{a}$ . Here, the dimension  $n = 2r$  is even, and  $\mathbb{R}^{2r}$  is endowed with the standard symplectic structure:

$$(5) \quad \omega(x, y) = \sum_{i=1}^r x_i y_{r+i} - x_{r+i} y_i,$$

and a vector field  $a = \sum_{i=1}^{2r} a_i \partial_i$  is hamiltonian if there exists a smooth map  $H : \mathbb{R}^{2r} \rightarrow \mathbb{R}$  such that:

$$\begin{aligned} a_i &= -\frac{\partial H}{\partial t_{i+r}} \text{ for } i = 1, \dots, r, \text{ and} \\ a_i &= \frac{\partial H}{\partial t_{i-r}} \text{ for } i = r+1, \dots, 2r. \end{aligned}$$

Recall that the Poisson bracket of two smooth maps  $f, g$  on  $\mathbb{R}^{2r}$  is given by:

$$(6) \quad \{f, g\} = \sum_{i=1}^r \frac{\partial f}{\partial t_i} \frac{\partial g}{\partial t_{i+r}} - \frac{\partial g}{\partial t_i} \frac{\partial f}{\partial t_{i+r}}.$$

Hence hamiltonian vector fields are those vector fields  $a$  which can be expressed as:

$$a = \{H, -\}$$

for some  $H \in C^\infty(\mathbb{R}^{2r})$ . A B-series turns out to be canonical if and only if the following condition holds for any rooted trees  $s$  and  $t$  [3, Theorem 2]:

$$(7) \quad \alpha(s \circ t) + \alpha(t \circ s) = \alpha(s)\alpha(t),$$

where  $s \circ t$  is the right Butcher product, defined by grafting the tree  $t$  on the root of the tree  $s$ . This result is also valid in the coloured case. The infinitesimal counterpart of this result expresses as follows ([16], Theorem IX.9.10 for one-colour case): a B-series  $B_{\underline{a}}(\alpha, -)$  with  $\alpha(\mathbf{1}) = 0$  defines a hamiltonian vector field for any hamiltonian vector field  $a$  if and only if:

$$(8) \quad \alpha(s \circ t) + \alpha(t \circ s) = 0.$$

Let us call the B-series of the type described above *hamiltonian B-series*. Our interest in non-rooted trees comes from the following elementary observation: the two rooted trees  $s \circ t$  and  $t \circ s$  are equal as non-rooted trees, and one is obtained from the other by shifting the root to a neighbouring vertex. As an easy consequence of (8), any hamiltonian B-series  $B_{\underline{a}}(\alpha, -)$  has to satisfy that if two rooted trees  $s$  and  $t$  are equal as non-rooted trees, then:

$$(9) \quad \alpha(s) = \pm \alpha(t).$$

This implies that, modulo a careful account of the signs involved, hamiltonian B-series are naturally indexed by non-rooted trees rather than by rooted ones. The sign is plus or minus according to the parity of the minimal number of "root shifts"  $s_1 \circ s_2 \mapsto s_2 \circ s_1$  that are required to change  $s$  into  $t$ .

In the present paper we address the following question: *what survives from the pre-Lie structure at the level of non-rooted trees?* There is a natural linear map  $\tilde{X}$  from non-rooted trees to (the linear span of) rooted trees, sending a tree to the sum of all its rooted representatives, with alternating signs. Its precise definition involves a total order on rooted trees introduced by A. Murua [19]. We propose a binary product  $\diamond$  on the linear span of non-rooted trees, which is roughly speaking an alternating sum of all trees obtained by linking a vertex of the first tree with a vertex of the second tree. Theorem 4 is the key result of the paper. It implies the fact that  $\diamond$  is a Lie bracket and that  $\tilde{X}$  is a Lie algebra morphism, the Lie bracket on rooted trees being given by antisymmetrizing the pre-Lie product.

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## 2. STRUCTURAL FACTS ABOUT NON-ROOTED TREES

We denote by  $T$  (resp.  $FT$ ) the set of non-planar rooted (resp. non-rooted) trees. We denote by  $\mathcal{T}$  (resp.  $\mathcal{FT}$ ) the vector spaces freely generated by  $T$  (resp.  $FT$ ). The projection  $\pi : T \twoheadrightarrow FT$  is defined by forgetting the root. It extends linearly to  $\pi : \mathcal{T} \twoheadrightarrow \mathcal{FT}$ . Rooted trees will be denoted by latin letters  $s, t, \dots$ , non-rooted trees by greek letters  $\sigma, \tau, \dots$ . We will also use "free tree" as a synonymous for "non-rooted tree". For any free tree  $\tau$  and for any vertex  $v$  of  $\tau$ , we denote by  $\tau_v$  the unique rooted tree built from  $\tau$  by putting the root at  $v$ .

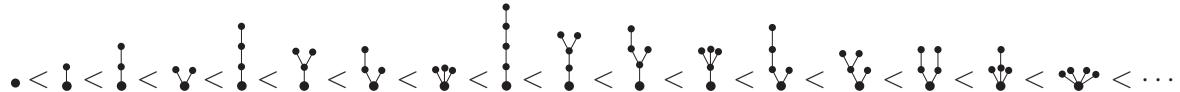
**2.1. A total order on rooted trees.** Recall that any rooted tree  $t$  is obtained by grafting rooted trees  $t_1, \dots, t_q$  on a common root:

$$t = B_+(t_1, \dots, t_q).$$

The trees  $t_j$  are called the *branches* of  $t$ . A. Murua defines in [19] a total order on the set of (one-colour) rooted trees in a recursive way as follows: the *canonical decomposition* of a tree  $t$  is given by  $t = t_L \circ t_R$  where  $t_R$  is the maximal branch of  $t$ . The maximality is to be understood with respect to the total order, supposed to be already defined for trees with number of vertices strictly smaller than  $|t|$ . Then  $s < t$  if and only if:

- either  $|s| < |t|$ ,
- or  $|s| = |t|$  and  $s_L < t_L$ ,
- or  $|s| = |t|$ ,  $s_L = t_L$  and  $s_R < t_R$ .

In the one-colour case, the total order of the first few trees is:



If we prescribe a total order on the set of colours  $D$  and allow the set of one node coloured trees to inherit this order, incorporating this into the definition above gives a total order on the set of coloured rooted trees. Note that the structure of the one-colour order is not entirely preserved,

as, for example, for two colours  $\bullet < \circ$  we have  $\bullet > \circ$  whereas  $\bullet < \circ$ .

**2.2. Superfluous trees.** This notion has been introduced in [1], where the authors describe order conditions for canonical B-series coming from Runge-Kutta approximation methods. Let  $B_{\underline{a}}(\alpha, -)$  be a hamiltonian B-series. According to (8), we have  $\alpha(t \circ t) = 0$  for any rooted tree  $t$ . Any non-rooted tree  $\tau$  such that there exists a rooted tree  $s$  with  $s \circ s \in \pi^{-1}(\tau)$  is called a *superfluous tree*, and a rooted tree  $t$  is said to be superfluous if its underlying free tree  $\pi(t)$  is. Such trees never appear in a hamiltonian B-series. For any free tree  $\tau \in FT$ , its *canonical representative* is the maximal element of the set  $\pi^{-1}(\tau) \subset T$  for the total order above. The following lemma gives a characterization of superfluous trees:

**Lemma 1.** *Let  $\tau \in FT$  have two distinct vertices  $v$  and  $w$  such that  $\tau_v = \tau_w$  is the canonical representative of  $\tau$ . Then:*

- (1)  *$v$  and  $w$  are the two ends of a common edge in  $\tau$ ,*
- (2) *There exists  $s \in T$  such that  $\tau_v = \tau_w = s \circ s$ .*

*Proof.* First of all, the maximal branch of  $\tau_v$  contains  $w$  (and vice-versa). Indeed, Suppose the maximal branch of  $\tau_v$  does not contain  $w$  (and hence vice-versa). Let

$$\tau_v = B^+(t_1, t_2, \dots, t_n, t_w, t_{\max}), \quad \tau_w = B^+(t'_1, t'_2, \dots, t'_n, t'_v, t'_{\max}),$$

where  $t_w$  is the branch of  $\tau_v$  containing  $w$  and  $t'_v$  similarly. It is clear that  $t'_v$  contains all branches of  $\tau_v$  except  $t_w$ . Hence  $|t'_v| > |t_1| + \dots + |t_n| + |t_{\max}|$  and as  $|t_{\max}| = |t'_{\max}|$  we have  $|t'_v| > |t'_{\max}|$ , a contradiction. Now suppose that  $v$  and  $w$  are not neighbours, and choose a vertex  $x$  between  $v$  and  $w$ , i.e. such that there is a path from  $v$  to  $w$  meeting  $x$ . The maximal branch of  $\tau_x$  cannot contain both  $v$  and  $w$ ; suppose it does not contain  $v$ . Then it is a subtree of the maximal branch  $\tau_v$  and hence contains strictly less vertices. Looking at the canonical decompositions:

$$t := \tau_v = \tau_w = t_L \circ t_R, \quad t' := \tau_x = t'_L \circ t'_R,$$

we have then  $|t'_L| > |t_L|$ , which immediately yields  $\tau_x > \tau_v$ , which is a contradiction. This proves the first assertion, and the second assertion follows immediately.  $\square$

There are four superfluous free trees with six vertices or less. The corresponding superfluous rooted trees are:



We denote by  $S$  the set of superfluous free trees and by  $FT'$  the set of non-superfluous trees, hence  $FT = FT' \amalg S$ . The corresponding linear spans will be denoted by  $\mathcal{S}$  and  $\mathcal{FT}'$ . We have  $\mathcal{FT} = \mathcal{S} \oplus \mathcal{FT}'$ , which leads to a linear isomorphism:

$$\mathcal{FT}' \sim \mathcal{FT}/\mathcal{S}.$$

**2.3. Symmetries.** We keep the notations of the previous subsection. For any non-superfluous tree  $\tau \in FT'$  we denote by  $*$  the unique vertex such that  $\tau_*$  is the canonical representative of  $\tau$ . The group of automorphisms of  $\tau$  is the subgroup  $\text{Aut } \tau$  of the group of permutations  $\varphi$  of  $\mathcal{V}(\tau)$  which respect the tree structure, i.e. such that, for any  $v, w \in \mathcal{V}(\tau)$ , there is an edge between  $v$  and  $w$  if and only if there is an edge between  $\varphi(v)$  and  $\varphi(w)$ .

For any rooted tree  $t$  we also denote by  $\text{Aut } t$  its group of automorphisms, i.e. the subgroup of the group of permutations  $\varphi$  of  $\mathcal{V}(t)$  which respect the rooted tree structure. It obviously coincides with the stabilizer of the root in  $\text{Aut } \pi(t)$ . Now for any non-superfluous free tree  $\tau$  it is obvious from Lemma 1 that  $\text{Aut } \tau$  fixes the vertex  $*$ , hence  $\text{Aut } \tau = \text{Aut } \tau_*$ .

Now  $\text{Aut } \tau$  acts on the set of vertices  $\mathcal{V}(\tau)$ . Moreover, for any vertex  $v$  this group acts transitively on the subset of possible roots for  $\tau_v$ , namely:

$$\mathcal{R}_v(\tau) := \{w \in \mathcal{V}(\tau), \tau_w \sim \tau_v\}.$$

Hence  $R_v(\tau)$  identifies itself with the homogeneous space:

$$(10) \quad R_v(\tau) \sim \text{Aut } \tau_*/\text{Aut } \tau_v.$$

This immediately leads to the following proposition, which is implicit in the proof of Lemma IX.9.7 in [16]:

**Proposition 2.** *Let  $\tau$  be a non-superfluous free tree, let  $t$  be a rooted tree such that  $\pi(t) = \tau$ , and let  $N(t, \tau)$  be the number of vertices  $v \in \mathcal{V}(\tau)$  such that  $\tau_v = t$ . Then:*

$$(11) \quad N(t, \tau) = \frac{\text{sym}(\tau_*)}{\text{sym}(t)}.$$

**2.4. Grafting and linking.** Let  $\sigma$  and  $\tau$  be two non-rooted trees, and let us choose a vertex  $v$  of  $\sigma$  and a vertex  $w$  of  $\tau$ . We will denote by  $\sigma_v \text{---}_w \tau$  the non-rooted tree obtained by taking  $\sigma$  and  $\tau$  together and adding a new edge between  $v$  and  $w$ . This linking operation is related to grafting of rooted trees as follows: for any other choice of vertices  $x$  of  $\sigma$  and  $y$  of  $\tau$  we have:

$$(12) \quad (\sigma_v \text{---}_w \tau)_y = \sigma_v \rightarrow_w \tau_y,$$

$$(13) \quad (\sigma_v \text{---}_w \tau)_x = \tau_w \rightarrow_v \sigma_x.$$

### 3. A BINARY OPERATION ON NON-ROOTED TREES

The linear map  $\tilde{X} : \mathcal{FT} \rightarrow \mathcal{T}$  is defined for any non-rooted tree  $\tau$  by:

$$(14) \quad \tilde{X}(\tau) = \sum_{v \in \mathcal{V}(\tau)} \varepsilon(v, \tau) \tau_v,$$

and extended linearly. Here  $\varepsilon(v, \tau)$  is equal to 0 if  $\tau$  is superfluous, and is equal to 1 (resp.  $-1$ ) if  $\tau$  is not superfluous and if the number of requested root shifts to change  $\tau_v$  into the canonical representative of  $\tau$  is even (resp. odd). This number, which we denote by  $\kappa(v, \tau)$ , is indeed unambiguous for non-superfluous trees according to Lemma 1. We obviously have:

$$(15) \quad \varepsilon(v, \tau) = \varepsilon(\varphi(v), \tau)$$

for any  $\varphi \in \text{Aut } \tau$ . The introduction of the map  $\tilde{X}$  is justified by the fact that, according to (8), (15) and Proposition 2, rooted trees involved in hamiltonian B-series do group themselves under terms  $\tilde{X}(\tau)$  with  $\tau \in \mathcal{FT}$ . Indeed,

**Proposition 3.**

$$(16) \quad B_{\underline{a}}(\alpha, -) = \sum_{\tau \in \mathcal{FT}} h^{|\tau|} \frac{\alpha(\tau_*)}{\text{sym}(\tau_*)} \mathcal{F}_{\underline{a}}(\tilde{X}(\tau)).$$

Now let us define a binary product on  $\mathcal{FT}$  by the formula:

$$(17) \quad \sigma \diamond \tau = \sum_{v \in \mathcal{V}(\sigma), w \in \mathcal{V}(\tau)} \delta(v, w) \sigma_v \text{---}_w \tau,$$

with  $\delta(v, w) := \varepsilon(w, \sigma_v \text{---}_w \tau) \varepsilon(v, \sigma) \varepsilon(w, \tau)$ .

**Theorem 4.** *We have  $\sigma \diamond \tau \in \mathcal{FT}'$  for any  $\sigma, \tau \in \mathcal{FT}$ , and  $\sigma \diamond \tau = 0$  if  $\sigma$  or  $\tau$  is superfluous. The product  $\diamond$  is antisymmetric, and the following relation holds:*

$$(18) \quad \tilde{X}(\sigma \diamond \tau) = \tilde{X}(\sigma) \rightarrow \tilde{X}(\tau) - \tilde{X}(\tau) \rightarrow \tilde{X}(\sigma) = [\tilde{X}(\sigma), \tilde{X}(\tau)].$$

*Proof.* A computation of the left-hand side gives:

$$\begin{aligned}\tilde{X}(\sigma \diamond \tau) &= \sum_{v,x \in \mathcal{V}(\sigma), w \in \mathcal{V}(\tau)} \varepsilon(x, \sigma_v \rightarrow_w \tau) \varepsilon(w, \sigma_v \rightarrow_w \tau) \varepsilon(v, \sigma) \varepsilon(w, \tau) (\sigma_v \rightarrow_w \tau)_x \\ &+ \sum_{v \in \mathcal{V}(\sigma), w, y \in \mathcal{V}(\tau)} \varepsilon(y, \sigma_v \rightarrow_w \tau) \varepsilon(w, \sigma_v \rightarrow_w \tau) \varepsilon(v, \sigma) \varepsilon(w, \tau) (\sigma_v \rightarrow_w \tau)_y,\end{aligned}$$

and computing the right-hand side gives:

$$\begin{aligned}[\tilde{X}(\sigma), \tilde{X}(\tau)] &= - \sum_{v,x \in \mathcal{V}(\sigma), w \in \mathcal{V}(\tau)} \varepsilon(v, \sigma) \varepsilon(w, \tau) \tau_w \rightarrow_x \sigma_v \\ &+ \sum_{v \in \mathcal{V}(\sigma), w, y \in \mathcal{V}(\tau)} \varepsilon(v, \sigma) \varepsilon(w, \tau) \sigma_v \rightarrow_y \tau_w.\end{aligned}$$

Exchanging  $x$  and  $v$  in the first sum, and  $y$  and  $w$  in the second, we get:

$$\begin{aligned}[\tilde{X}(\sigma), \tilde{X}(\tau)] &= - \sum_{v,x \in \mathcal{V}(\sigma), w \in \mathcal{V}(\tau)} \varepsilon(x, \sigma) \varepsilon(w, \tau) \tau_w \rightarrow_v \sigma_x \\ &+ \sum_{v \in \mathcal{V}(\sigma), w, y \in \mathcal{V}(\tau)} \varepsilon(v, \sigma) \varepsilon(y, \tau) \sigma_v \rightarrow_w \tau_y.\end{aligned}$$

The first assertion is immediate since  $\varepsilon(w, \sigma_v \rightarrow_w \tau)$  vanishes if  $\sigma_v \rightarrow_w \tau$  is superfluous. The second assertion is also immediate, since  $\delta(v, w)$  vanishes if  $\sigma$  or  $\tau$  is superfluous. The antisymmetry comes from the fact that  $v$  and  $w$  are neighbours in  $\sigma_v \rightarrow_w \tau$ .

- (1) If  $\sigma$  or  $\tau$  is superfluous, any individual term in both sides vanishes.
- (2) If  $\sigma$  and  $\tau$  are not superfluous it may happen that  $\sigma_v \rightarrow_w \tau$  is superfluous for some  $v \in \mathcal{V}(\sigma)$  and  $w \in \mathcal{V}(\tau)$ . The corresponding term  $\tilde{X}(\sigma_v \rightarrow_w \tau)$  in  $\tilde{X}(\sigma \diamond \tau)$  vanishes. On the other hand, the sum of all terms in  $[\tilde{X}(\sigma), \tilde{X}(\tau)]$  corresponding to the couple  $(v, w)$  chosen above writes down as:

$$\begin{aligned}T_{v,w} &:= - \sum_{x \in \mathcal{V}(\sigma)} (-1)^{\kappa(x, \sigma) + \kappa(w, \tau)} \tau_w \rightarrow_v \sigma_x \\ &+ \sum_{y \in \mathcal{V}(\tau)} (-1)^{\kappa(v, \sigma) + \kappa(y, \tau)} \sigma_v \rightarrow_w \tau_y.\end{aligned}$$

The distance  $d(x, v)$  between  $x$  and  $v$  in  $\sigma$  is defined as the length of the (unique) path joining  $x$  and  $v$  in  $\sigma$ . It is clearly equal modulo 2 to the sum  $\kappa(x, \sigma) + \kappa(v, \sigma)$ . Similarly,  $d(y, w) = \kappa(y, \tau) + \kappa(w, \tau)$  modulo 2. Hence, using (12) and (13) we get:

$$T_{v,w} = (-1)^{\kappa(v, \sigma) + \kappa(w, \tau)} \left( - \sum_{x \in \mathcal{V}(\sigma)} (-1)^{d(x, v)} (\sigma_v \rightarrow_w \tau)_x + \sum_{y \in \mathcal{V}(\tau)} (-1)^{d(y, w)} (\sigma_v \rightarrow_w \tau)_y \right).$$

Now the distance  $d(x, v)$  is the same if we compute it in  $\sigma$  or in  $\sigma_v \rightarrow_w \tau$ , and similarly for  $d(y, w)$ . Finally, using the fact that  $v$  and  $w$  are neighbours in  $\sigma_v \rightarrow_w \tau$ , we have  $d(x, w) = d(x, v) + 1$  for any  $x \in \mathcal{V}(\sigma)$ , the distance being computed in  $\sigma_v \rightarrow_w \tau$ . This finally gives:

$$T_{v,w} = (-1)^{\kappa(v, \sigma) + \kappa(w, \tau)} \sum_{z \in \mathcal{V}(\sigma_v \rightarrow_w \tau)} (-1)^{d(z, w)} (\sigma_v \rightarrow_w \tau)_z,$$

which vanishes since  $\sigma_v \rightarrow_w \tau$  is superfluous.

- (3) Finally, if  $\sigma, \tau$  and  $\sigma_v - w\tau$  are not superfluous, using (12) and (13), both sides will be equal if we have:

$$\begin{aligned}\kappa(x, \sigma_v - w\tau) + \kappa(w, \sigma_v - w\tau) + \kappa(v, \sigma) &= \kappa(x, \sigma) + 1 \text{ modulo } 2, \\ \kappa(y, \sigma_v - w\tau) + \kappa(w, \sigma_v - w\tau) + \kappa(w, \tau) &= \kappa(y, \tau) \text{ modulo } 2.\end{aligned}$$

Using the fact that  $v$  and  $w$  are neighbours, it rewrites as:

$$\begin{aligned}\kappa(x, \sigma_v - w\tau) + \kappa(x, \sigma) &= \kappa(v, \sigma_v - w\tau) + \kappa(v, \sigma) \text{ modulo } 2, \\ \kappa(y, \sigma_v - w\tau) + \kappa(y, \tau) &= \kappa(w, \sigma_v - w\tau) + \kappa(w, \tau) \text{ modulo } 2.\end{aligned}$$

These two last identities are always verified: looking for example at the right-hand side of the first one, moving vertex  $v$  to a neighbour will change both  $\kappa$ 's by  $\pm 1$ . It remains then to jump from neighbour to neighbour up to  $x$ . The proof of the second identity is completely similar.  $\square$

Using the identification of  $\mathcal{FT}/\mathcal{S}$  with  $\mathcal{FT}'$ , a straightforward consequence of Theorem 4 is the following:

**Corollary 5.** *The linear map  $\tilde{X}$  is an injection of  $\mathcal{FT}'$  into  $\mathcal{T}$ , and the product  $\diamond : \mathcal{FT}' \times \mathcal{FT}' \rightarrow \mathcal{FT}'$  verifies:*

$$\tilde{X}(\sigma \diamond \tau) = [\tilde{X}(\sigma), \tilde{X}(\tau)].$$

As a consequence, the product  $\diamond$  satisfies the Jacobi identity, and  $\tilde{X}$  is an embedding of Lie algebras.

#### 4. APPLICATION TO ELEMENTARY HAMILTONIANS

Keeping the previous notations, the vector field  $\mathcal{F}_{\underline{a}}(\tilde{X}(\tau))$  is hamiltonian for any (decorated) non-rooted tree  $\tau$ . Hence it can be uniquely written as  $\{H_{\underline{a}}(\tau), -\}$  for some  $H_{\underline{a}}(\tau) \in C^\infty(\mathbb{R}^{2r})$ , called the *elementary hamiltonian* associated with  $\tau$ .

**Proposition 6.** *For any free trees  $\sigma, \tau$  we have:*

$$(19) \quad \{H_{\underline{a}}(\sigma), H_{\underline{a}}(\tau)\} = H_{\underline{a}}(\sigma \diamond \tau).$$

*Proof.* We compute:

$$\begin{aligned}\{\{H_{\underline{a}}(\sigma), H_{\underline{a}}(\tau)\}, -\} &= [\{H_{\underline{a}}(\sigma), -\}, \{H_{\underline{a}}(\tau), -\}] \\ &= [\mathcal{F}_{\underline{a}}(\tilde{X}(\sigma)), \mathcal{F}_{\underline{a}}(\tilde{X}(\tau))] \\ &= \mathcal{F}_{\underline{a}}([\tilde{X}(\sigma), \tilde{X}(\tau)]) \\ &= \mathcal{F}_{\underline{a}} \circ \tilde{X}(\sigma \diamond \tau) \\ &= \{H_{\underline{a}}(\sigma \diamond \tau), -\}.\end{aligned}$$

One concludes by using the uniqueness of the hamiltonian representation of a hamiltonian vector field.  $\square$

#### REFERENCES

- [1] L. Abia, J. M. Sanz-Serna, *Order conditions for canonical Runge-Kutta schemes*, SIAM J. Numer. Anal. **28**, 1081-1096 (1991).
- [2] A. Agrachev, R. Gamkrelidze, *Chronological algebras and nonstationary vector fields*, J. Sov. Math. 17 (1981) 1650–1675.
- [3] A. L. Araujo, A. Murua, J.-M. Sanz-Serna, *Symplectic methods based on decompositions*, SIAM J. Num. Anal. (1996).

- [4] Ch. Brouder, *Runge-Kutta methods and renormalization*, Eur. Phys. J. C Part. Fields 12 (2000) 512–534.
- [5] J. C. Butcher, *An algebraic theory of integration methods*, Math. Comp. 26 (1972) 79–106.
- [6] J. C. Butcher, *The numerical analysis of ordinary differential equations. Runge-Kutta and general linear methods*, Wiley, Chichester, 2008.
- [7] M. P. Calvo, J. M. Sanz-Serna, *Canonical B-series*, Numer. Math. 67, 161–175 (1994).
- [8] A. Cayley, *On the theory of the analytical forms called trees*, Phil. Mag. 13, 172–176 (1857).
- [9] E. Celledoni, R. McLachlan, D. McLaren, B. Owren, R. Quispel W. Wright, *Energy-preserving Runge-Kutta methods*, M2AN (Mathematical Modelling and Numerical Analysis), 43 (4), 645–649 (2009).
- [10] F. Chapoton, M. Livernet, *Pre-Lie algebras and the rooted trees operad*, Internat. Math. Res. Notices 2001 (2001) 395–408.
- [11] F. Chapoton, M. Livernet, *Relating two Hopf algebras built from an operad*, Internat. Math. Res. Notices 2007 Art. ID rnm131, 27 pp.
- [12] Ph. Chartier, E. Hairer, G. Vilmart, *A substitution law for B-series vector fields*, preprint INRIA No. 5498 (2005).
- [13] Ph. Chartier, E. Hairer, G. Vilmart, *Numerical integrators based on modified differential equations*, Math. Comp. 76 (2007) 1941–1953.
- [14] Ph. Chartier, A. Murua, *An algebraic theory of order*, M2AN Math. Model. Numer. Anal. 43 (2009) 607–630.
- [15] A. Dzhumadil'daev, C. Löfwall, *Trees, free right-symmetric algebras, free Novikov algebras and identities*, Homology Homotopy and Appl. 4 (2002) 165–190.
- [16] E. Hairer, C. Lubich, G. Wanner, *Geometric numerical integration Structure-preserving algorithms for ordinary differential equations*, vol. 31, Springer Series in Computational Mathematics. Springer-Verlag, Berlin, 2002.
- [17] D. Kreimer, *The combinatorics of (perturbative) quantum field theories*, Phys. Rep. 363 (2002) 387–424. [arXiv:hep-th/0010059](https://arxiv.org/abs/hep-th/0010059)
- [18] H. Munthe-Kaas, W. Wright, *On the Hopf Algebraic Structure of Lie Group Integrators*, Found. Comput. Math. 8 (2008) 227–257.
- [19] A. Murua, *The Hopf algebra of rooted trees, free Lie algebras, and Lie series*, Found. Comput. Math. 6 (2006) 387–426.
- [20] J.-M. Sanz-Serna, *Runge-Kutta schemes for hamiltonian systems*, BIT Numerical Analysis, 28 No4 (1988), 877–883.
- [21] J. M. Sanz-Serna, *Symplectic integrators for Hamiltonian problems: an overview*, Acta Numerica 1(1992), 243–286.

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