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**Milnor invariants of braids and welded braids up to homotopy**

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# Milnor invariants of braids and welded braids up to homotopy

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We consider the group of pure welded braids (also known as loop braids) up to (link-)homotopy. The pure welded braid group classically identifies, via the Artin action, with the group of basis-conjugating automorphisms of the free group, also known as the McCool group  $P\Sigma_n$ . It has been shown recently that its quotient by the homotopy relation identifies with the group  $hP\Sigma_n$  of basis-conjugating automorphisms of the reduced free group. We describe a decomposition of this quotient as an iterated semidirect product which allows us to solve the Andreadakis problem for this group, and to give a presentation by generators and relations. The Andreadakis equality can be understood, in this context, as a statement about Milnor invariants; a discussion of this question for classical braids up to homotopy is also included.

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Introduction	1277
0. Reminders: strongly central series and Lie rings	1281
1. The reduced free group and its Lie algebra	1284
2. Derivations and the Johnson morphism	1290
3. The Andreadakis problem	1294
4. Topological interpretation	1303
5. A presentation of the homotopy loop braid group	1306
Appendix. Lyndon words and the free Lie algebra	1311
References	1318

## Introduction

The present paper is a contribution to the theory of loop braids (also called *welded braids*), via the study of their finite-type invariants. Finite-type invariants were defined by Vassiliev [1990] and were much studied during the 1990s (see for instance [Gusarov 1994; Kontsevich 1993]), giving birth to a whole field of research, which is still very active nowadays. Finite-type invariants of string-links and braids have been the focus of several papers in the late 1990s, by Stanford [1996; 1998], Mostovoy and Willerton [2002], and Habegger and Masbaum [2000]. By then, finite-type invariants of braids were fairly well understood. Meanwhile, a generalization of finite-type invariants to virtual knotted objects was introduced in [Gusarov et al. 2000]. However, it was only much later that this definition was used and studied for welded knotted

objects [Bar-Natan and Dancso 2016; 2017]. In the meantime, the interest for welded knotted objects had grown, as the link between welded diagrams, four-dimensional topology and automorphisms of the free group had become more apparent [Baez et al. 2007; Fenn et al. 1997; Satoh 2000]; see [Damiani 2017] for a survey of welded braids. In recent years, the study of these objects has been flourishing; see for instance [Audoux 2016; Bardakov and Bellingeri 2014; Damiani 2019; Kamada 2007; Meilhan and Yasuhara 2019; Nakamura et al. 2018]. In particular, link-homotopy for these objects (corresponding to self-virtualization moves in welded diagrams) has been the focus of several recent papers [Audoux et al. 2017a; 2017b; Audoux and Meilhan 2019].

The invariants under scrutiny in this paper appear naturally as filtrations on groups. Precisely, suppose  $G$  is a group whose elements are the objects one is interested in. For example, these could be mapping classes of a manifold, automorphisms of a group, (welded) braids up to isotopy, (welded) braids up to homotopy, etc. Suppose we are also given a filtration of  $G$  by subgroups:  $G = G_1 \supseteq G_2 \supseteq \dots$ . Then one can consider the class  $[g]_d$  of an element  $g \in G$  inside  $G/G_{d+1}$  and hope to understand  $g$  through its approximations  $[g]_d$ , which become finer and finer as  $d$  grows to infinity. These approximation are often easier to understand than  $g$ . For instance,  $[g]_d$  could be described by a finite family of integers (or other simple mathematical objects), that we would call *invariants of degree at most  $d$* .

With this point of view, the question of comparing different filtrations on the same group (such as the Andreadakis problem — see Section 0.1) can be interpreted as a problem of comparison between different kinds of invariants. Conversely, comparing different notions of invariants on elements of a group can often be interpreted as a problem of comparison between different filtrations on the group, provided that these invariants are indexed by some kind of degree measuring their accuracy, and that they possess some compatibility with the group structure. It is mainly the latter point of view that we adopt below, working with filtrations on groups, with a rather algebraic point of view, getting back to the language of invariants only to interpret our results. This is motivated by the fact that the invariants we consider are strongly compatible with the group structures: not only do they come from filtrations by subgroups, as described above, but these filtrations are *strongly central*, a very nice property allowing us to study them using Lie algebras. Moreover, all the filtrations we consider do have a natural algebraic definition.

We consider mainly three kinds of filtrations (or invariants):

- **Minor invariants** correspond to *Andreadakis-like filtrations* (or the Johnson filtration for the mapping class group). These are defined for automorphism groups of groups, and their subgroups.
- **Finite-type (or Vassiliev) invariants** with coefficients in a fixed commutative ring  $\mathbb{k}$  correspond to the *dimension filtration*  $D_*^{\mathbb{k}}G = G \cap (1 + I^*)$ , where  $I$  is the augmentation ideal of the group ring  $\mathbb{k}G$ .
- **The lower central series** on  $G$  is the minimal strongly central filtration on  $G$ .

The minimality of the lower central series means that the corresponding invariants of degree  $d$  contain as much information as possible for invariants possessing this compatibility with the group structure. Since

the two other filtrations are also strongly central, and the Milnor invariants are of finite type, the above list goes from the coarsest invariants to the finest ones. Thus, although we will not always emphasize this in the sequel, the reader should keep in mind that a statement of the form “Milnor invariants of degree at most  $d$  distinguish classes of elements  $g \in G$  modulo  $\Gamma_{d+1}G$ ” implies that Milnor invariants of degree at most  $d$  are universal finite-type invariants of degree at most  $d$ , and that finite-type invariants of degree at most  $d$  distinguish classes of elements  $g \in G$  modulo  $\Gamma_{d+1}G$ .

## Main results

We are interested in the group of pure welded braids (or pure welded string-links) up to homotopy. This group identifies, through a version of the Artin action up to homotopy, with the group  $hP\Sigma_n$  of (pure) basis-conjugating automorphisms of the *reduced free group*  $RF_n$  (see [Definition 1.2](#)). The key result of this paper is the decomposition theorem:

**Theorem 3.1** *There is a decomposition of  $hP\Sigma_n$  into a semidirect product*

$$hP\Sigma_n \cong \left[ \left( \prod_{i < n} \mathcal{N}(x_n)/x_i \right) \rtimes (RF_n/x_n) \right] \rtimes hP\Sigma_{n-1},$$

where  $\mathcal{N}(x_n)/x_i$  is the normal closure of  $x_n$  inside  $RF_n/x_i$ , and the action of  $RF_n/x_n \cong RF_{n-1}$  on the product is the diagonal one. Moreover, the semidirect product on the right is an almost direct one.

The reduced free group is studied in [Section 1](#). In particular, using the version of the Magnus expansion for the reduced free groups introduced by Milnor, which takes values in the *reduced free algebra*, we are able to show an analogue of Magnus’s theorem:

**Theorem 1.12** *The Lie ring of the reduced free group identifies with the **reduced free Lie algebra** on the same set of generators.*

The restriction  $hP\Sigma_n \cap \mathcal{A}_*(RF_n)$  of the Andreadakis filtration  $\mathcal{A}_*(RF_n)$  of  $RF_n$  encodes Milnor invariants of pure welded braids. We are able to determine the structure of the associated graded Lie algebra in [Section 2.1](#):

**Theorem 2.9** *The Lie algebra  $\mathcal{L}(hP\Sigma_n \cap \mathcal{A}_*(RF_n))$  identifies, via the Johnson morphism, to the algebra of **tangential derivations** of the reduced free algebra.*

On the other hand, the decomposition of  $hP\Sigma_n$  ([Theorem 3.1](#)) induces a decomposition of its lower central series, which in turn gives a decomposition of the associated Lie algebra ([Theorem 3.8](#)). We are thus able to compare the lower central series and the Andreadakis filtrations via a comparison of their associated graded Lie algebras, getting the promised comparison result, which we also show for the group  $hP_n$  of classical pure braids up to homotopy, embedded into  $\text{Aut}(RF_n)$  via the Artin action:

**Theorem 3.9** *The Andreadakis equality holds for  $G = hP_n$  and  $G = hP\Sigma_n$ ; that is,*

$$G \cap \mathcal{A}_*(RF_n) = \Gamma_*G.$$

In other words, Milnor invariants of degree at most  $d$  classify braids up to homotopy (resp. welded braids up to homotopy) up to elements of  $\Gamma_{d+1}(hP_n)$  (resp.  $\Gamma_{d+1}(hP\Sigma_n)$ ).

Notice that there is no obvious link between this theorem and its analogue up to isotopy. On the one hand, for classical braids up to isotopy, the fact that Milnor invariants can detect the lower central series of  $P_n$  has been known for a long time [Habegger and Masbaum 2000; Mostovoy and Willerton 2002], but the result up to homotopy is new, and cannot be deduced from the former (as far as I know). On the other hand, for (pure) welded braids (that is, for basis-conjugating automorphisms of the free group), the result up to isotopy is still open. In fact, although [Bardakov 2003, Theorem 1] gives a decomposition of  $P\Sigma_n$  similar to our decomposition theorem (see also Remarks 3.4 and 3.6), the pieces of this decomposition are poorly understood, far from the fairly complete description in our setting. Besides, one feature of  $hP_n$  and  $hP\Sigma_n$  which makes them very different from  $P_n$  and  $P\Sigma_n$  (and in fact, much easier to handle) is their *nilpotence*, which is used throughout the paper.

Finally, we use our methods to give a presentation of the group  $hP\Sigma_n$ . A classical result of McCool [1986] asserts that the group  $P\Sigma_n$  of (pure) basis-conjugating automorphisms of the free group  $F_n$  is the group generated by generators  $\chi_{ij}$  ( $i \neq j$ ) submitted to the *McCool relations*:

$$\begin{aligned} [\chi_{ik}\chi_{jk}, \chi_{ij}] &= 1 \quad \text{for } i, j, k \text{ pairwise distinct,} \\ [\chi_{ik}, \chi_{jk}] &= 1 \quad \text{for } i, j, k \text{ pairwise distinct,} \\ [\chi_{ij}, \chi_{kl}] &= 1 \quad \text{if } \{i, j\} \cap \{k, l\} = \emptyset. \end{aligned}$$

We show that we need to add three families of relation to get its quotient  $hP\Sigma_n$ :

**Theorem 5.8** *The pure loop braid group up to homotopy  $hP\Sigma_n$  is the group generated by generators  $\chi_{ij}$  ( $i \neq j$ ) submitted to the McCool relations on the  $\chi_{ij}$ , and the three families of relations,*

$$[\chi_{mi}, w, \chi_{mi}] = [\chi_{im}, w, \chi_{jm}] = [\chi_{im}, w, \chi_{mi}] = 1,$$

for  $i, j < m, i \neq j$ , and  $w \in \langle \chi_{mk} \rangle_{k < m}$ .

The method used for the group can be adapted to the Lie algebra associated to the lower central series of  $hP\Sigma_n$ . We show in Section 5.3 that it admits a similar presentation. We also give a presentation of the Lie algebra of  $hP_n$  in Corollary 3.12.

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## 0 Reminders: strongly central series and Lie rings

We give here a short introduction to the theory of strongly central filtrations and their associated Lie rings, whose foundations were laid by M Lazard [1954]. Details may be found in [Darné 2019; 2021].

### 0.1 A very short introduction to the Andreadakis problem

Let  $G$  be an arbitrary group. The left and right action of  $G$  on itself by conjugation are denoted respectively by  $x^y = y^{-1}xy$  and  ${}^yx = yxy^{-1}$ . The *commutator* of two elements  $x$  and  $y$  in  $G$  is  $[x, y] := xyx^{-1}y^{-1}$ . If  $A$  and  $B$  are subsets of  $G$ , we denote by  $[A, B]$  the subgroup generated by all commutators  $[a, b]$  with  $(a, b) \in A \times B$ . We denote the *abelianization* of  $G$  by  $G^{\text{ab}} := G/[G, G]$  and its lower central series by  $\Gamma_*(G)$ ; that is,

$$G = \Gamma_1(G) \supseteq [G, G] = \Gamma_2(G) \supseteq [G, \Gamma_2(G)] = \Gamma_3(G) \supseteq \dots$$

The lower central series is a fundamental example of a *strongly central filtration* (or  $N$ -series) on a group  $G$ :

**Definition 0.1** A *strongly central filtration*  $G_*$  on a group  $G$  is a nested sequence of subgroups

$$G = G_1 \supseteq G_2 \supseteq G_3 \supseteq \dots$$

such that  $[G_i, G_j] \subseteq G_{i+j}$  for all  $i, j \geq 1$ .

In fact, the lower central series is the minimal such filtration on a given group  $G$ , as is easily shown by induction.

Recall that when  $G_*$  is a strongly central filtration, the quotients  $\mathcal{L}_i(G_*) := G_i/G_{i+1}$  are abelian groups, and the whole graded abelian group  $\mathcal{L}(G_*) := \bigoplus G_i/G_{i+1}$  is a Lie ring (ie a Lie algebra over  $\mathbb{Z}$ ), where Lie brackets are induced by group commutators. The lower central series of a group is usually difficult to understand, but we are often helped by the fact that its associated Lie algebra is always generated in degree one.

**Convention 0.2** If  $g$  is an element of a group  $G$  endowed with a (strongly central) filtration  $G_*$ , the *degree of  $g$  with respect to  $G_*$*  is the minimal integer  $d$  such that  $g \in G_d - G_{d+1}$ . Since most of the filtrations we consider satisfy  $\bigcap G_i = \{1\}$ , this is well defined (if not, we could just say that  $d = \infty$  for elements of  $\bigcap G_i$ ). We often speak of *the class  $\bar{g}$  of  $g$  in the Lie algebra  $\mathcal{L}(G_*)$* , by which we mean the only nontrivial one, in  $\mathcal{L}_d(G_*) = G_d/G_{d+1}$ , where  $d$  is the degree of  $g$  with respect to  $G_*$ , unless a fixed degree is specified.

When  $G_*$  is a strongly central filtration on  $G = G_1$ , there is a universal way of defining a strongly central filtration on a group of automorphisms of  $G$ . Precisely, we get a strongly central filtration on a subgroup of  $\text{Aut}(G_*)$ , the latter being the group of automorphisms of  $G$  preserving the filtration  $G_*$ :

$$(0-1) \quad \mathcal{A}_j(G_*) := \{\sigma \in \text{Aut}(G_*) \mid \forall i \geq 1, [\sigma, G_i] \subseteq G_{i+j}\}.$$

The commutator is computed in  $G \rtimes \text{Aut}(G)$ , which means that for  $\sigma \in \text{Aut}(G)$  and  $g \in G$ ,  $[\sigma, g] = \sigma(g)g^{-1}$ . Thus,  $\mathcal{A}_j(G_*)$  is the group of automorphisms of  $G_*$  acting trivially on the quotients  $G_i/G_{i+j}$  ( $i \geq 1$ ). For instance,  $\mathcal{A}_1(G_*)$  is the group of automorphisms of  $G_*$  acting trivially on  $\mathcal{L}(G_*)$ . When  $G_*$  is the lower central series of a group  $G$ , then  $\mathcal{L}(G) := \mathcal{L}(\Gamma_*(G))$  is generated (as a Lie ring) by  $\mathcal{L}_1(G) = G^{\text{ab}}$ , so  $\mathcal{A}_1(G)$  identifies with the group  $IA_G$  of automorphisms of  $G$  acting trivially on its abelianization  $G^{\text{ab}}$ . Thus  $\mathcal{A}_*(G) := \mathcal{A}_*(\Gamma_*(G))$  is a strongly central filtration on  $IA_G$ , and we can try to understand how it compares to the minimal such filtration on  $IA_G$ , which is its lower central series:

**Problem 1** (Andreadakis) *For a given group  $G$ , how close is the inclusion of  $\Gamma_*(IA_G)$  into  $\mathcal{A}_*(G)$  to being an equality?*

One way to attack this problem is to restrict to subgroups of  $IA_G$ . Precisely, if  $K \subseteq IA_G$  is a subgroup, we can consider the following three strongly central filtrations on  $K$ :

$$\Gamma_*(K) \subseteq K \cap \Gamma_*(IA_G) \subseteq K \cap \mathcal{A}_*(G).$$

**Definition 0.3** We say that the *Andreadakis equality* holds for a subgroup  $K$  of  $IA_G$  when

$$\Gamma_*(K) = K \cap \mathcal{A}_*(G).$$

Our three main tools in calculating Lie algebras are the following:

**Lazard’s theorem [1954, Theorem 3.1]** (see also [Darné 2019, Theorem 1.36]) If  $A$  is a filtered ring (that is,  $A$  is filtered by ideals  $A = A_0 \supseteq A_1 \supseteq A_2 \supseteq \dots$  such that  $A_i A_j \subseteq A_{i+j}$ ), the subgroup  $A^\times \cap (1 + A_1)$  of  $A^\times$  inherits a strongly central filtration  $A_*^\times := A^\times \cap (1 + A_*)$  whose Lie ring embeds into the graded ring  $\text{gr}(A_*)$ , via

$$\mathcal{L}(A_*^\times) \hookrightarrow \text{gr}(A_*), \quad \bar{x} \mapsto \overline{x-1}.$$

If  $G$  is any group endowed with a morphism  $\alpha: G \rightarrow A^\times$ , then we can pull the filtration  $A_*^\times$  back to  $G$ , and  $\mathcal{L}(\alpha^{-1}(A_*^\times))$  embeds into  $\mathcal{L}(A_*^\times)$ , thus into  $\text{gr}(A_*)$ .

**Semidirect product decompositions [Darné 2021, Section 3.1]** If  $G_*$  is a strongly central filtration,  $G_* = H_* \rtimes K_*$  is a *semidirect product of strongly central filtrations* if  $G_i = H_i \rtimes K_i$  is a semidirect product of groups for all  $i$ , and  $[K_i, H_j] \subseteq H_{i+j}$  for all  $i$  and  $j$ . Then the strong centrality of  $G_*$  implies that  $H_*$  and  $K_*$  must be strongly central. This kind of decomposition is useful because it induces a decomposition of Lie algebras

$$\mathcal{L}(G_*) = \mathcal{L}(H_*) \rtimes \mathcal{L}(K_*).$$

Now, if  $G = H \rtimes K$  is any semidirect product of groups, then its lower central series decomposes into a semidirect product  $\Gamma_*(G) = \Gamma_*^K(H) \rtimes \Gamma_*(K)$  of strongly central filtrations, where  $\Gamma_*^K(H)$  is defined by

$$H = \Gamma_1^K(H) \supseteq [G, H] = \Gamma_2^K(H) \supseteq [G, \Gamma_2^K(H)] = \Gamma_3^K(H) \supseteq \dots$$

When the semidirect product is an *almost-direct* one, which means that  $K$  acts trivially on  $H^{\text{ab}}$ , then  $\Gamma_*^K(H) = \Gamma_*(H)$ , so in this case

$$\mathcal{L}(H \rtimes K) = \mathcal{L}(H) \rtimes \mathcal{L}(K).$$

**The Johnson morphism [Darné 2019, Section 1.4]** A very useful tool to study a filtration of the form  $\mathcal{A}_*(G_*)$  is the Johnson morphism, which encodes the fact that the associated graded Lie algebra  $\mathcal{L}(\mathcal{A}_j(G_*))$  acts faithfully on the graded Lie algebra  $\mathcal{L}(G_*)$ . It is defined by

$$\tau: \mathcal{L}(\mathcal{A}_*(G_*)) \hookrightarrow \text{Der}(\mathcal{L}(G_*)), \quad \bar{\sigma} \mapsto \overline{[\sigma, -]},$$

which means that it is induced by  $\sigma \mapsto (x \mapsto \sigma(x)x^{-1})$ . Its injectivity comes from the universality of the filtration  $\mathcal{A}_*(G_*)$ .

If we want to compare the filtration  $\mathcal{A}_*(G_*)$  with another one, we can do so using comparison morphisms. For example, if  $K$  is a subgroup of  $\text{Aut}(G_*)$ , the inclusion of  $\Gamma_*K$  into  $K \cap \mathcal{A}_*(G_*)$  induces a morphism  $i_*: \mathcal{L}(K) \rightarrow \mathcal{L}(K \cap \mathcal{A}_*(G_*))$  which is injective if and only if  $\Gamma_*K = K \cap \mathcal{A}_*(G_*)$ . Thus we can show the Andreadakis equality by showing the injectivity of the morphism  $\tau' := \tau \circ i_*$  ( $\tau'$  is also sometimes called the Johnson morphism).

## 0.2 The case of the free group

Before beginning our study of the Andreadakis problem for the reduced free group, it may be useful to recall some basic facts about the free group case. Here  $F_n$  denotes the free group on  $n$  generators  $x_1, \dots, x_n$ .

**Magnus expansions** The assignment  $x_i \mapsto 1 + X_i$  defines an embedding of  $F_n$  into the group of invertible power series on  $n$  noncommuting indeterminates  $X_1, \dots, X_n$  with integral coefficients. In fact, it is easy to see that it defines a morphism to  $1 + (X_1, \dots, X_n)$ , and that this induces (using universal properties) an isomorphism of completed rings,

$$\widehat{\mathbb{Z}F_n} \cong \widehat{T[n]},$$

where the group ring  $\mathbb{Z}F_n$  is completed with respect to the filtration by the powers of its augmentation ideal, and the tensor algebra  $T[n]$  on  $n$  generators  $X_1, \dots, X_n$  is completed with respect to the usual valuation. One shows that the above morphism from  $F_n$  to this ring is injective by showing directly that the image of a reduced nontrivial word must be nontrivial.

**Magnus’s theorem** Using Lazard’s theorem, we can get a surjection of  $\mathcal{L}(F_n)$  onto the Lie ring generated in degree one inside  $\text{gr}(\widehat{T[n]}) \cong T[n]$ , which is the free Lie ring  $\mathcal{L}[n]$  on  $n$  generators. Using freeness, one shows that this surjection has to be injective as well;

$$\mathcal{L}(F_n) \cong \mathcal{L}[n].$$

**The Andreadakis problem and the Johnson morphism** In the case of the free group, the Johnson morphism defines an embedding of  $\mathcal{L}(\mathcal{A}_*(F_n))$  into the Lie ring of derivations of the free Lie ring.



The Andreadakis problem for automorphisms of free groups is a difficult problem. The two filtrations were first conjectured to be equal [Andreadakis 1965, page 253]. This was disproved very recently [Bartholdi 2016], but the methods used do not give a good understanding of what is going on. The Andreadakis equality is known to hold for certain well-behaved subgroups, such as the pure braid group  $P_n$  [Darné 2021; Satoh 2017]. However, the problem stays largely open in general. In particular, it is open for the group  $P\Sigma_n$  of basis-conjugating automorphisms (that is, for the group of pure welded braids), of which our group  $hP\Sigma_n$  is a simpler version.

## 1 The reduced free group and its Lie algebra

In this first section, we introduce and study the *reduced free group*, which was first introduced by Milnor [1954] as the link group of the trivial link with  $n$  components. Using the Magnus expansion defined in [Milnor 1954], we determine its Lie ring.

**Notation 1.1** Several of our constructions are functors on the category of sets. For such a functor  $\Phi$ , we denote by  $\Phi[X]$  its value at a set  $X$ . When  $X$  is finite with  $n$  elements, we will often denote  $\Phi[X]$  by  $\Phi[n]$  or by  $\Phi_n$ .

### 1.1 The reduced free group

**Definition 1.2** The *reduced free group* on a set  $X$  is the group defined by the presentation

$$\text{RF}[X] := \langle X \mid \forall x \in X, \forall w \in F[X], [x, x^w] = 1 \rangle.$$

This means that it is the largest group generated by  $X$  such that each element of  $X$  commutes with all its conjugates.

Since any  $x$  commutes with itself, the relations  $[x, x^w]$  of Definition 1.2 can also be written  $[x, [x, w]]$ . The next result and its proof are taken from [Habegger and Lin 1990, Lemma 1.3]:

**Proposition 1.3** For any integer  $n$ , the group  $\text{RF}_n$  is  $n$ -nilpotent. For any set  $X$ , the group  $\text{RF}[X]$  is residually nilpotent.

**Proof** We use the fact that  $\text{RF}[-]$  is a functor on pointed sets. First, for a finite set  $X$ , we show by induction on  $n = |X|$  that  $\text{RF}_n = \text{RF}[X]$  is  $n$ -nilpotent. This is obvious for  $n = 1$ , because  $\text{RF}_1 \cong \mathbb{Z}$ . Suppose that  $\text{RF}_{n-1}$  is  $(n-1)$ -nilpotent. If  $x \in X$ , the normal subgroup  $\mathcal{N}(x)$  of  $\text{RF}[X]$  generated by  $x$  is the kernel of the projection  $p_x$  from  $\text{RF}[X]$  to  $\text{RF}[X - \{x\}]$  sending  $x$  to 1. We have an exact sequence

$$1 \rightarrow \bigcap_{x \in X} \mathcal{N}(x) \rightarrow \text{RF}[X] \xrightarrow{p=(p_x)} \prod_{x \in X} \text{RF}[X - \{x\}].$$

Since the group on the right is  $(n-1)$ -nilpotent by the induction hypothesis, the morphism  $p$  must send  $\Gamma_n(\text{RF}[X])$  to 1, so that  $\Gamma_n(\text{RF}[X])$  is inside the kernel  $\bigcap \mathcal{N}(x)$ . Moreover, by definition of the reduced

free group, for every  $x \in X$ , all elements of  $\mathcal{N}(x)$  commute with  $x$ . Thus, an element of  $\bigcap \mathcal{N}(x)$  commutes with all  $x \in X$ , so it is in the center  $\mathcal{Z}(\mathbf{RF}[X])$ . As a conclusion,  $\Gamma_n(\mathbf{RF}[X]) \subseteq \mathcal{Z}(\mathbf{RF}[X])$ , which means exactly that  $\mathbf{RF}[X]$  is  $n$ -nilpotent.

Suppose now  $X$  infinite. Let  $w$  be an element of  $\mathbf{RF}[X]$ . It can be written as a product of a finite number of elements of  $X$  and their inverses. Denote by  $W$  such a finite subset of  $X$ . Then  $w$  is inside the image of the canonical injection  $\mathbf{RF}[W] \hookrightarrow \mathbf{RF}[X]$ , which is split by the projection from  $\mathbf{RF}[X]$  to  $\mathbf{RF}[W]$  sending  $X - W$  to 1. Since  $\mathbf{RF}[W]$  is  $|W|$ -nilpotent, this construction provides a nilpotent quotient of  $\mathbf{RF}[X]$  in which the image of  $w$  is nontrivial, whence the residual nilpotence of  $\mathbf{RF}[X]$ .  $\square$

## 1.2 The reduced free algebra

**Definition 1.4** Let  $Y$  be a set. If  $s \geq 2$  is an integer, let us define  $\Delta_s(Y)$  by

$$\Delta_s(Y) := \{(y_i) \in Y^s \mid \exists i \neq j, y_i = y_j\}.$$

The *reduced free algebra* on  $Y$  is the unitary associative ring defined by the presentation

$$A[Y] := \langle Y \mid \forall s, \forall (y_i) \in \Delta_s(Y), y_1 \cdots y_s = 0 \rangle.$$

For short, we often forget the mention of  $Y$  when it is clear from the context, and write only  $A$  for  $A[Y]$ .

**Fact 1.5** The algebra  $A[Y]$  is graded by the degree of monomials. As a  $\mathbb{Z}$ -module,  $A[Y]$  is a direct factor of the tensor algebra  $T[Y]$ ; a (finite) basis of  $A[Y]$  is given by **monomials without repetition** on the generators  $y \in Y$ , which are monomials of the form  $y_1 \cdots y_s$  with  $(y_i) \notin \Delta_s(Y)$ .

**Proof** Let  $R$  be the (free)  $\mathbb{Z}$ -submodule of  $T[Y]$  generated by the  $y_1 \cdots y_s$  such that  $(y_i) \in \Delta_s(Y)$  (monomials *with repetition*). This module is clearly a homogeneous ideal of  $T[Y]$ . As a consequence,  $A = T/R$ . Moreover, if we denote by  $S$  the (free)  $\mathbb{Z}$ -submodule of  $T$  generated by monomials without repetition, then  $T = S \oplus R$  as a  $\mathbb{Z}$ -module, so  $A \cong S$ .  $\square$

**Definition 1.6** Let  $Y$  be a set. The *reduced free Lie algebra* on  $Y$  is the Lie algebra defined by the presentation

$$R\mathcal{L}[Y] := \langle Y \mid \forall s, \forall (y_i) \in \Delta_s(Y), [y_1, \dots, y_s] = 0 \rangle,$$

where  $[y_1, \dots, y_s]$  denotes  $[y_1, [y_2, [\dots [y_{s-1}, y_s] \dots]]]$ .

The following result uses some of the combinatorics of the free Lie ring recalled in the [appendix](#):

**Proposition 1.7** The Lie subalgebra of  $A[Y]$  generated by  $Y$  identifies with  $R\mathcal{L}[Y]$ .

**Proof** We need to prove that the intersection of the ideal  $R$  of relations defining  $A[Y]$  with the free Lie algebra  $\mathcal{L}[Y] \subset T[Y]$  is exactly the module  $S$  of relations defining  $R\mathcal{L}[Y]$ . The inclusion of  $S$  into  $R$  is

clear: when we decompose a relation in  $S$  on the basis of  $TV$ , only monomials with exactly the same letters appear, counting repetitions. For the converse, let us first remark that thanks to [Lemma A.14](#),  $S$  is the submodule of  $\mathcal{L}[Y]$  generated by all Lie monomials with repetition. Let  $p \neq 0$  be an element of  $R \cap \mathcal{L}[Y]$ , and let us consider its decomposition  $p = \sum \lambda_w P_w$  on the Lyndon basis of  $\mathcal{L}[Y]$ . Let  $w$  be the smallest Lyndon word such that  $\lambda_w \neq 0$ . It follows from [Lemma A.7](#) that  $\lambda_w$  must be the coefficient of  $w$  in the decomposition of  $p$  into a linear combination of monomials of  $TV$ . Since  $p \in R$ , the word  $w$  must be with repetition, so  $P_w \in S$ . Then  $p - \lambda_w P_w \in R \cap \mathcal{L}[Y]$  has less terms than  $p$  in its decomposition on the Lyndon basis, giving us the result by induction.  $\square$

**Remark 1.8** When  $Y$  is a finite set with  $n$  elements, we can extract finite presentations from the above presentations. Indeed, the ideal  $R$  and the Lie ideal  $S$  are both generated in degrees at most  $n + 1$ , since  $R_{n+1} = T[n]_{n+1}$  and  $S_{n+1} = \mathcal{L}[n]_{n+1}$  (a word of length  $n + 1$  must possess at least a repetition). As a consequence, the relations of degree at most  $n + 1$  are enough to describe  $A[n]$  (resp.  $R\mathcal{L}[n]$ ), and there are finitely many of them.

**Proposition 1.9** *Lyndon monomials without repetition on the  $y_i$  are a basis of  $R\mathcal{L}[Y]$ . The rank of the degree- $k$  part  $R\mathcal{L}[n]_k$  of  $R\mathcal{L}[n]$  is  $(k - 1)! \binom{n}{k}$ .*

**Proof** [Lemma A.14](#) implies that the module  $S$  in the proof of [Proposition 1.7](#) is the submodule generated by all Lyndon monomials with repetition, which are thus a basis of  $S$ . As a consequence, Lyndon monomials without repetition give a basis of the quotient  $R\mathcal{L}[Y] = \mathcal{L}[Y]/S$ .

In order to determine the ranks, we need to count Lyndon words without repetition of length  $k$  in  $y_1, \dots, y_n$ . A word without repetition is Lyndon if and only if its first letter is the smallest one. Such a word is determined by the choice of  $k$  letters, and a choice of ordering of the  $(k - 1)$  letters left when the smallest one is removed. This gives  $(k - 1)! \binom{n}{k}$  such words, as announced.  $\square$

**Proposition 1.10** *In  $A[Y]^\times$ , each element of  $1 + Y$  commutes with all its conjugates.*

**Proof** Let  $y$  be an element of  $Y$ . From the relation  $y^2 = 0$ , we deduce that  $1 + y$  is invertible, with  $1 - y$  as its inverse. Let  $u \in A^\times$ . Then  $u(1 + y)u^{-1} = 1 + yuu^{-1}$ . Since  $yAy = 0$ , we can write

$$(1 + y)(1 + yuu^{-1}) = 1 + y + yuu^{-1} = (1 + yuu^{-1})(1 + y),$$

which is the desired conclusion.  $\square$

**Notation 1.11** From now on, we denote by  $X$  and  $Y$  two sets endowed with a bijection  $X \cong Y$  that we will denote by  $x_i \mapsto y_i$  (we consider both  $X$  and  $Y$  indexed by a bijection from a set of indices  $I$ ). This notation will allow us to distinguish between the group-theoretic world and its algebraic counterpart.

From [Proposition 1.10](#), we get a well-defined morphism, which is an analogue of the Magnus expansion, and was introduced by Milnor [[1954](#), Section 4],

$$(1-1) \quad \mu: \text{RF}[X] \rightarrow A[Y]^\times, \quad x_i \mapsto 1 + y_i.$$

From Lazard's theorem [1954, Theorem 3.1] (see also [Darné 2019, Theorem 1.36]), we get an associated morphism between graded Lie algebras,

$$(1-2) \quad \bar{\mu}: \mathcal{L}(\text{RF}[X]) \rightarrow \text{gr}(A[Y]) \cong A[Y], \quad \bar{x}_i \mapsto y_i.$$

From this we deduce our first main theorem:

**Theorem 1.12** *The above morphism (1-2) induces a canonical isomorphism between the Lie algebra of the reduced free group and the reduced free algebra,*

$$\mathcal{L}(\text{RF}[X]) \cong R\mathcal{L}[Y].$$

**Proof** Since  $\mathcal{L}(\text{RF}[X])$  is generated in degree 1 [Darné 2019, Proposition 1.19] (that is, generated by the  $\bar{x}_i$ ), the morphism (1-2) defines a surjection from  $\mathcal{L}(\text{RF}[X])$  onto the Lie subalgebra of  $A$  generated by  $Y$ , which is  $R\mathcal{L}[Y]$  (Proposition 1.7). But  $\mathcal{L}(\text{RF}[X])$  is a reduced Lie algebra on  $X$ , by which we mean that the relations on the  $y_i$  defining  $R\mathcal{L}[Y]$  are true for the classes  $\bar{x}_i$ . Indeed, in  $\text{RF}[X]$ , the normal closure  $\mathcal{N}(x)$  of a generator  $x \in X$  is commutative. As a consequence, if  $u$  is any element of  $\mathcal{N}(x)$ , then  $[x, u] = 1$ . Applying this to  $u = [x_{r+1}, \dots, x_s, x, w] \in \mathcal{N}(x)$  (where our notation for iterated commutators is the same as above for iterated brackets in Lie algebras), we see that any  $[x_1, \dots, x_r, x, x_{r+1}, \dots, x_s, x, w]$  is trivial in the group, hence so is its class in the Lie algebra. Thus  $y_i \mapsto \bar{x}_i$  defines an inverse to our surjection, which has to be an isomorphism.  $\square$

**Corollary 1.13** *The morphism  $\mu: x_i \mapsto 1 + y_i$  (1-1) from  $\text{RF}[X]$  to  $A[Y]^\times$  is injective.*

**Proof** Let  $w$  be an element of  $\ker(\mu)$ . If  $w \neq 1$ , then, by residual nilpotence of  $\text{RF}[X]$  (Proposition 1.3), there exists an integer  $k$  such that  $w \in \Gamma_k - \Gamma_{k+1}$ . Thus,  $\bar{w}$  is a nontrivial element of  $\mathcal{L}_k(\text{RF}[X])$ , sent to 0 by  $\bar{\mu}$ . But  $\bar{\mu}$  is an isomorphism (Theorem 1.12), so this is not possible; our element  $w$  must be trivial.  $\square$

**Remark 1.14** This statement also appears in [Bar-Natan 1995]; compare Proposition 5.2 therein.

**Some remarks on finite presentations of nilpotent groups** Every nilpotent group of finite type admits a finite presentation. This fact is easy to prove, by induction on the nilpotency class, using that finitely generated abelian groups are finitely presented, and that an extension of finitely presented groups is finitely presented. As a consequence, the reduced free group  $\text{RF}_n$  on  $x_1, \dots, x_n$  must admit a finite presentation. Can we find a simple one? Considering that we have a finite presentation of the associated Lie algebra, the problem does not seem to be difficult, at first glance. Indeed, let  $G_n$  is the group admitting the same finite presentation as  $R\mathcal{L}_n$  (see Remark 1.8), where brackets are replaced by commutators. These relations are true in  $\text{RF}_n$  (see the proof of Theorem 1.12), thus there is a map  $\pi$  from  $G_n$  onto  $\text{RF}_n$ , which must induce an isomorphism at the level of Lie rings. However, we can deduce that  $\pi$  is an isomorphism *only if we know that both these groups are nilpotent*. Which raises the question: do the relations defining  $G_n$  imply that it is nilpotent?

Thus we are led to ask ourselves: *what finite set of relation is needed to ensure that a group is nilpotent?* This question is strongly related to the following question: *can we give a simple finite presentation of the free nilpotent group of class  $c$*  (where “simple” is taken in some naive sense)?. This question is surprisingly difficult. The reader can convince himself that killing commutators of the form  $[x_{i_0}, \dots, x_{i_c}]$  (or even  $[x_{i_0}^{\pm}, \dots, x_{i_c}^{\pm}]$ ) does not seem to be enough, because the usual formulas of commutator calculus seem not to allow one to reduce to commutators of this particular form and length. Even killing all iterated commutators of length  $c + 1$  of the generators is only conjectured to be enough [Jackson 2008; Sims 1987].

To get a presentation known to work in general, we must take a much larger one. For instance, one can kill all iterated commutators of the generators of length between  $c + 1$  and  $2c$ . This can be improved slightly by killing only relations of the form  $[x, y]$ , where  $x$  and  $y$  are iterated commutators of the generators of length at most  $c$ , whose length add up to at least  $c + 1$ . Indeed, all iterated commutators of length greater than  $c$  can be written as a product of conjugates of iterated commutators of the generators of length greater than  $c$  (by repeated use of the formulas  $[a, bc] = [a, b] \cdot [a, c] \cdot [[c, a], b]$  and  $[a, b^{-1}] = [b, a]^b$ ). And every such commutator has a subcommutator of the given form (to see that, it can help to think of commutator words as rooted planar binary trees).

In order to avoid these problems, and to keep our presentations simple, we will only give a presentation of  $\text{RF}_n$  as a nilpotent group, that is, we assume that the group  $G_n$  in the reasoning above is nilpotent, thus obtaining:

**Proposition 1.15** *The reduced free group  $\text{RF}_n$  is the quotient of the free  $n$ -nilpotent group on  $x_1, \dots, x_n$  by the finite set of relations*

$$\forall s \leq n \quad \forall (x_i) \in \Delta_s(X) \quad [x_1, \dots, x_s] = 1,$$

where  $[x_1, \dots, x_s]$  denotes  $[x_1, [x_2, [\dots [x_{s-1}, x_s] \dots ]]]$ .

The subtlety of this situation was not perceived in [Cohen 1995], where it was assumed that this presentation (with  $n + 1$  commutators included) would automatically define a nilpotent group. Note that several results of the present paper give some insight on the group-theoretic results of [Cohen 1995], which were stated only in terms of the underlying abelian groups, and become simpler when taking into account the Lie ring structure.

### 1.3 Centralizers

We will use Corollary 1.13 to compute the centralizers of generators in  $\text{RF}[X]$ . First, we show a lemma about commutation relations in  $A[Y]$ :

**Lemma 1.16** *Let  $y \in Y$ , and let  $\lambda$  be an integer. Define the  $\lambda$ -centralizer  $C_\lambda(y)$  of  $y$  in  $A[Y]$  to be*

$$C_\lambda(y) := \{u \in A[Y] \mid uy = \lambda yu\}.$$

If  $\lambda \neq 1$ , then  $C_\lambda(y)$  is exactly  $\langle y \rangle$ . If  $\lambda = 1$ , then  $C_\lambda(y) = \mathbb{Z} \cdot 1 \oplus \langle y \rangle$ . As a consequence,  $\mathbb{Z} \cdot 1 \oplus \langle y \rangle$  is the centralizer  $C(y)$  of  $y$ . Also,  $\langle y \rangle$  is the annihilator  $\text{Ann}(y)$  of  $y$ , and it is also the set of elements  $u$  satisfying  $uy = -yu$ .

**Proof** If  $u$  is an element of  $\langle y \rangle$ , then  $uy = \lambda yu = 0$ . Moreover, obviously,  $1 \in C_1(y)$ . This proves one inclusion. Let us prove the converse. Let  $u$  be an element of  $C_\lambda(y)$ . Let us decompose  $u$  as a sum of monomials without repetition  $\sum \lambda_\alpha m_\alpha$  in  $A$ , and consider a monomial  $m_\alpha \neq 1$  not containing  $y$ . Then  $\lambda_\alpha$  is the coefficient of  $m_\alpha y$  in  $0 = uy - \lambda yu$ , so it must be zero. Also, if  $\mu$  is the coefficient of  $1$  in  $m$ , then the coefficient of  $y$  in  $uy - \lambda yu$  is  $(1 - \lambda)\mu$ , hence  $\mu = 0$  if  $\lambda \neq 1$ . Thus all the monomials appearing in the decomposition of  $u$  (except possibly  $1$  if  $\lambda = 1$ ) must contain  $y$ , so that  $u$  belongs to  $\langle y \rangle$  (resp. to  $\mathbb{Z} \oplus \langle y \rangle$  if  $\lambda = 1$ ).  $\square$

The next lemma is [Habegger and Lin 1990, Lemma 1.10]:

**Lemma 1.17** *Let  $x \in X$ . Let  $C(x)$  be the centralizer of  $x$  in  $\text{RF}[X]$ . Then  $C(x)$  is exactly the normal closure  $\mathcal{N}(x)$  of  $x$ .*

**Proof** The inclusion  $\mathcal{N}(x) \subseteq C(x)$  follows from the definition of  $\text{RF}[X]$ . Let us prove the converse. From Corollary 1.13, we know that  $C(x) = C(1 + y) \cap \text{RF}[X] = (\mathbb{Z} \oplus \langle y \rangle) \cap \text{RF}[X]$ . Moreover,  $\text{RF}[X] \hookrightarrow A[Y]$  takes values in  $1 + \bar{A}[Y]$  (where  $\bar{A}$  is the augmentation ideal of  $A$ , that is, the set of polynomials with no constant term). As a consequence, this intersection is  $(1 + \langle y \rangle) \cap \text{RF}[X]$ . But  $1 + \langle y \rangle$  is exactly the set of elements sent to  $1$  by the projection  $A[Y] \rightarrow A[Y - \{y\}]$ . This projection induces the projection from  $\text{RF}[X]$  to  $\text{RF}[X - \{x\}]$ , whose kernel is  $\mathcal{N}(x)$ , whence the result.  $\square$

**Lemma 1.18** *Let  $y \in Y$ . Let  $C_{\mathcal{L}}(y)$  be the centralizer of  $y$  in  $R\mathcal{L}[Y]$ . Then  $C_{\mathcal{L}}(y)$  is exactly the Lie ideal  $\langle y \rangle$  generated by  $y$ .*

**Proof** If we now denote by  $\langle y \rangle_A$  the ideal generated by  $y$  in  $A$  (denoted by  $\langle y \rangle$  above), we have that  $C_{\mathcal{L}}(y) = C_1(y) \cap R\mathcal{L}[Y] = \langle y \rangle_A \cap R\mathcal{L}[Y]$  is the submodule of  $R\mathcal{L}[Y]$  generated by Lie monomials in which  $y$  appears, which is exactly  $\langle y \rangle$ .  $\square$

**Proposition 1.19** *The center of  $\text{RF}_n$  is the intersection of the  $\mathcal{N}(x_i)$ , and also coincides with  $\Gamma_n(\text{RF}_n)$ ; it is free abelian of rank  $(n - 1)!$*

**Proof** The inclusions  $\Gamma_n(\text{RF}_n) \subseteq \bigcap \mathcal{N}(x_i) \subseteq \mathcal{Z}(\text{RF}_n)$  were established in the proof of Proposition 1.3. Let  $w$  be a nontrivial element of  $\mathcal{Z}(\text{RF}_n)$ . Since  $\text{RF}_n$  is nilpotent,  $w \in \Gamma_k - \Gamma_{k+1}$  for some  $k$ , and  $\bar{w}$  is a nontrivial element in the center of  $\mathcal{L}(\text{RF}_n) \cong R\mathcal{L}_n$  (see Theorem 1.12). From Lemma 1.18, we deduce that  $\bar{w}$  is in the Lie ideal  $\langle y_1 \rangle \cap \dots \cap \langle y_n \rangle$ . As a consequence, all  $y_i$  appear at least once in each Lie monomial of the decomposition of  $\bar{w}$ . Thus its degree must be at least  $n$ , which means that  $w \in \Gamma_n(\text{RF}_n)$ .

Moreover,  $\Gamma_n(\text{RF}_n) = \Gamma_n(\text{RF}_n) / \Gamma_{n+1}(\text{RF}_n) = \mathcal{L}_n(\text{RF}_n)$  identifies with the degree- $n$  part  $R\mathcal{L}[n]_n$  of  $R\mathcal{L}[n]$ , which is free abelian of rank  $(n - 1)!$  by Proposition 1.9.  $\square$

## 2 Derivations and the Johnson morphism

In order to tackle the Andreadakis problem for  $\text{RF}_n$ , we need to understand the associated Johnson morphism, whose target is the algebra of derivations of the reduced free Lie algebra.

### 2.1 Derivations

We begin our study of derivations by those of  $A[Y]$ , which are quite easy to handle.

**Proposition 2.1** *Any derivation  $d$  of  $A[Y]$  sends each element  $y$  of  $Y$  to an element of the ideal  $\langle y \rangle$ . Conversely, any application  $d_Y : Y \rightarrow A[Y]$  sending each  $y$  into  $\langle y \rangle$  extends uniquely to a derivation of  $A[Y]$ .*

**Proof** First, given a derivation  $d$ , we can apply it to the relation  $y^2 = 0$ . We get that  $(dy)y + y(dy) = 0$ . Thus  $dy \in C_{-1}(y)$ , which means that  $dy \in \langle y \rangle$  by [Lemma 1.16](#).

Suppose now that we are given a map  $d_Y : Y \rightarrow A[Y]$  sending each  $y$  into  $\langle y \rangle$ . Then  $d_Y$  extends uniquely to a derivation  $d_T$  from  $T[Y]$  to  $A[Y]$  (the latter being a  $T[Y]$ -bimodule in the obvious sense) in the usual way,

$$d_T(y_{i_1} \cdots y_{i_l}) := \sum_{j=1}^l y_{i_1} \cdots y_{i_{j-1}} \cdot d_Y(y_{i_j}) \cdot y_{i_{j+1}} \cdots y_{i_l}.$$

From the hypothesis on  $d_Y$ , we deduce that  $d$  vanishes on the monomials with repetition (the sum on the left being a sum of monomials with repetition in this case), so it induces a well-defined derivation  $d : A[Y] \rightarrow A[Y]$  extending  $d_Y$ . Unicity is obvious from the fact that  $Y$  generates the ring  $A[Y]$ .  $\square$

We now turn to the study of derivations of  $R\mathcal{L}[Y]$ . We consider only derivations (strictly) increasing the degree, that is, sending  $Y$  into  $R\mathcal{L}[Y]_{\geq 2}$ . In fact, we will mostly be concerned with homogeneous such derivations (which raise the degree by a fixed amount), but we will see that this distinction is not important for  $R\mathcal{L}[Y]$  ([Corollary 2.3](#)).

**Proposition 2.2** *Let  $d$  be a derivation of  $R\mathcal{L}[Y]$ . Then for any  $y \in Y$ ,*

$$dy \in \langle y \rangle + \bigcap_{y' \neq y} \langle y' \rangle =: J_y,$$

where  $\langle y \rangle$  is the Lie ideal generated by  $y$ . Conversely, any map from  $Y$  to  $R\mathcal{L}[Y]_{\geq 2}$  satisfying this condition can be extended uniquely to a derivation of  $R\mathcal{L}[Y]$ .

Let us remark that the homogeneous ideal  $J_y$  differs from  $\langle y \rangle$  only in degree  $|Y| - 1$  (in particular, only when  $Y$  is finite), since the second term is generated by Lie monomials without repetition where all  $y'$  appear, save possibly  $y$ . Moreover, one easily sees that, for  $|Y| = n$ , the ideal  $J_y$  contains all of  $R\mathcal{L}[n]_{n-1}$ .



**Proof of Proposition 2.2** For  $|Y| = 2$ , remark that  $R\mathcal{L}[Y]_2 \subset \langle y_1 \rangle \cap \langle y_2 \rangle$  and  $R\mathcal{L}[Y]_{\geq 3} = \{0\}$ . As a consequence, any linear map raising the degree satisfies the condition and defines a derivation, so we have nothing to show.

Let us suppose that  $Y$  has at least three elements. Let  $d$  be a derivation of  $R\mathcal{L}[Y]$ , and let  $y \in Y$ . Take  $z \in Y - \{y\}$ , and consider the relation  $0 = d([y, z, y]) = [dy, z, y] + [y, z, dy]$ . Let us decompose  $dy$  as a sum of monomials in  $A[Y]$ . Let  $m$  be a monomial which contains neither  $y$  nor  $z$ , and let  $\lambda$  be the coefficient of  $m$  in  $dy$ . Then the monomial  $mzy$  appears with coefficient  $2\lambda$  in the decomposition of  $[dy, z, y] + [y, z, dy]$ , so  $\lambda$  must be trivial. Since this is true for any  $z \neq y$ , the only monomials without repetition not containing  $y$  that can appear in  $dy$  are the ones containing every element of  $Y$  save  $y$ , which are exactly the generators of  $J_y$  modulo  $\langle y \rangle$ . This shows that  $dy \in J_y$ .

To show the converse, we can restrict to homogeneous maps, since any map from  $Y$  to  $R\mathcal{L}[Y]_{\geq 2}$  is a sum of homogeneous ones, and a sum of derivations is a derivation. Suppose that we are given a homogeneous map  $d_Y : Y \rightarrow R\mathcal{L}[Y]_{\geq 2}$  sending each  $y$  into  $J_y$ . If  $d_Y$  is not of degree  $|Y| - 2$ , this condition amounts to  $d_Y(y) \in \langle y \rangle$ . This Lie ideal stands inside the associative ideal  $\langle y \rangle \subset A[Y]$ . We can thus use Proposition 2.1 to extend this map to a derivation of  $A[Y]$ . This derivation sends  $Y$  into  $R\mathcal{L}[Y]$ , hence it preserves  $R\mathcal{L}[Y] \subset A[Y]$ . As a consequence, it restricts to a derivation of  $R\mathcal{L}[Y]$  extending  $d_Y$ .

We are left to study the case when  $Y$  has  $n$  elements and  $d_Y$  is of degree  $n - 2$ . Then the conditions on the elements  $d_Y(y)$  are empty. We can still extend  $d_Y$  to a derivation from  $T[Y]$  to  $A[Y]$ , as in the proof of Proposition 2.1, but it does not vanish on the relations defining  $A[Y]$ . However, the induced Lie derivation from  $\mathcal{L}[Y]$  to  $R\mathcal{L}[Y]$  does vanish on the Lie monomials with repetition. Indeed, it vanishes on all elements of degree at least 3 (sent to  $R\mathcal{L}[Y]_{\geq n+1} = \{0\}$ ), and there are no such monomials in degree 2, since the elements  $[y, y]$  are already trivial in  $\mathcal{L}[Y]$ . As a consequence, it induces a well-defined derivation from  $R\mathcal{L}[Y]$  to itself. This derivation extends  $d_Y$  and is the only one to do so, since  $R\mathcal{L}[Y]$  is generated by  $Y$ . □

**Corollary 2.3** Any derivation of  $R\mathcal{L}_n$  is the sum of homogeneous components,

$$\text{Der}(\mathcal{L}_n) \cong \bigoplus_{k \geq 1} \text{Der}_k(R\mathcal{L}_n).$$

**Proof** If  $d$  is such a derivation, Proposition 2.2 shows that the homogeneous components of its restriction to  $Y$  extend uniquely to derivations of  $R\mathcal{L}_n$ , whose sum coincides with  $d$  on  $Y$ , hence everywhere. Note that it makes sense to speak of this sum, because  $Y$  is finite, so that the number of nontrivial homogeneous components of  $d|_Y$  is finite. □

The following theorem is an analogue of [Darné 2019, Proposition 2.41], replacing free nilpotent groups by reduced free groups.

**Theorem 2.4** Let  $n \geq 2$  be an integer. The Johnson morphism is an isomorphism:

$$\mathcal{L}(\mathcal{A}_*(\text{RF}_n)) \cong \text{Der}(R\mathcal{L}_n).$$



**Proof** Take  $|X| = |Y| = n$ . Let  $d$  be a derivation of  $R\mathfrak{L}[Y]$ , of degree  $k$ . We need to lift it to an automorphism  $\varphi$  of  $\text{RF}[X]$ . We first suppose that  $k \neq n - 2$ . Since  $d(y_i) \in \langle y_i \rangle \cap R\mathfrak{L}_{k+1}[Y]$  ([Proposition 2.2](#)), we can write each  $d(y_i)$  as a linear combination of Lie monomials of length  $k + 1$  containing  $y_i$ . The corresponding product of brackets in  $\text{RF}[X]$  lifts  $d(y_i)$  to an element  $w_i$  of  $\Gamma_{k+1}(\text{RF}[X]) \cap \mathcal{N}(x_i)$ . The element  $w_i x_i$  belongs to  $\mathcal{N}(x_i)$ , so it commutes with all its conjugates. As a consequence,  $x_i \mapsto w_i x_i$  defines an endomorphism  $\varphi$  of  $\text{RF}[X]$ . Since  $\varphi$  acts trivially on the abelianization of  $\text{RF}[X]$ , which is nilpotent, it is an automorphism [[Darné 2019](#), Lemma 2.38]. Moreover, by construction,  $\tau(\bar{\varphi}) = d$ .

Suppose now that  $k = n - 2$ . Then  $d(y_i)$  can be any element of  $R\mathfrak{L}_{n-1}[Y]$ . Choose any lift  $w_i$  in  $\Gamma_{n-1}(\text{RF}[X])$  of  $d(y_i)$ . Using the usual formulas of commutator calculus, we see that for any  $w \in \text{RF}[X]$ ,  $[w_i x_i, w, w_i x_i] \equiv [x_i, w, x_i] \pmod{\Gamma_{n+1}}$ . Since  $[x_i, w, x_i] = 1$  and  $\Gamma_{n+1}(\text{RF}_n) = \{1\}$ , we conclude that  $[w_i x_i, w, w_i x_i] = 1$ , which means exactly that  $w_i x_i$  commutes with all its conjugate. The same construction as in the first case then gives an automorphism  $\varphi \in \mathcal{A}_{n-2}$  such that  $\tau(\bar{\varphi}) = d$ . □

## 2.2 Tangential derivations

**Definition 2.5** A tangential derivation of  $R\mathfrak{L}[Y]$  is a derivation sending each  $y \in Y$  to an element of the form  $[y, w_y]$  (for some  $w_y \in R\mathfrak{L}[Y]$ ).

**Fact 2.6** The subset  $\text{Der}_\tau(R\mathfrak{L}[Y])$  of tangential derivations is a Lie subalgebra of  $\text{Der}(R\mathfrak{L}[Y])$ .

**Proof** Let  $d : y \mapsto [y, w_y]$  and  $d' : y \mapsto [y, w'_y]$ . Then an elementary calculation gives

$$(2-1) \quad [d, d'](y) = [y, [w_y, w'_y] + d(w'_y) - d'(w_y)],$$

whence the result. □

**Proposition 2.7** Let  $n \geq 2$  be an integer. The Lie subalgebra of  $\text{Der}(R\mathfrak{L}_n)$  generated in degree 1 is the subalgebra  $\text{Der}_\tau(R\mathfrak{L}_n)$  of tangential derivations.

**Proof** Consider the derivation  $d_{ij}$  sending  $y_i$  to  $[y_i, y_j]$  and all the other  $y_k$  to 0. From [Proposition 2.2](#), we know that these generate the module of derivations of degree 1. They are tangential derivations, so the Lie subalgebra they generate is inside  $\text{Der}_\tau(R\mathfrak{L}[Y])$ . Let us show that it is all of  $\text{Der}_\tau(R\mathfrak{L}[Y])$ . Consider the set  $D_i$  of tangential derivations sending all  $y_k$  to 0, save the  $i^{\text{th}}$  one. Such derivations vanish on all monomials which are not in  $\langle y_i \rangle$ , and preserve  $\langle y_i \rangle$ . Since elements of  $\langle y_i \rangle$  commute with  $y_i$ , formula (2-1) implies that

$$c_i : \mathfrak{R}\mathfrak{L}[Y] \rightarrow D_i, \quad t \mapsto (y_i \mapsto [y_i, t]),$$

is a morphism. It is obviously surjective, so  $D_i$  is a Lie subalgebra of  $\text{Der}_\tau(R\mathfrak{L}[Y])$ . Moreover, its kernel is  $\langle y_i \rangle$  ([Lemma 1.18](#)), so  $D_i \cong R\mathfrak{L}[Y]/y_i$  is in fact the free reduced Lie algebra on the  $c_i(y_j) = d_{ij}$  (for  $j \neq i$ ). Since  $\text{Der}_\tau(R\mathfrak{L}[Y])$  is the (linear) finite direct sum of the  $D_i$ , it is indeed generated (as a Lie algebra) by the  $d_{ij}$ . □

Recall that the *McCool group*  $P\Sigma_X$  is the group of automorphisms of the free group  $F[X]$  on a set  $X$  fixing the conjugacy class of each generator  $x \in X$ .

**Definition 2.8** The *reduced McCool group*  $hP\Sigma_X$  is the subgroup of  $\text{Aut}(\text{RF}[X])$  preserving the conjugacy class of each generator  $x \in X$  of  $\text{RF}[X]$ .

This group  $hP\Sigma_X$  is also called  $\text{Aut}_C(\text{RF}_X)$ , but we prefer to think of it as version of  $P\Sigma_X$  up to homotopy (this terminology will be explained in Section 4). When  $X$  is finite, we denote its elements by  $x_1, \dots, x_n$  and  $hP\Sigma_X$  by  $hP\Sigma_n$ .

Consider the filtration  $\mathcal{A}_*(\text{RF}_n)$  on  $\text{Aut}(\text{RF}_n)$ . It restricts to a filtration  $hP\Sigma_n \cap \mathcal{A}_*(\text{RF}_n)$  on  $hP\Sigma_X$ . Moreover, since  $\mathcal{A}_*(\text{RF}_n)$  is strongly central on the subgroup  $\mathcal{A}_1(\text{RF}_n)$  of automorphisms acting trivially on  $\text{RF}_n^{\text{ab}}$ , and  $hP\Sigma_n \subset \mathcal{A}_1(\text{RF}_n)$ , this induced filtration is strongly central on  $hP\Sigma_n$ .

**Theorem 2.9** Let  $n \geq 2$  be an integer. The Johnson morphism induces an isomorphism

$$\mathcal{L}(hP\Sigma_n \cap \mathcal{A}_*(\text{RF}_n)) \cong \text{Der}_\tau(R\mathcal{L}_n).$$

**Proof** Let  $\varphi: x_i \mapsto x_i^{w_i}$  be a basis-conjugating automorphism belonging to  $\mathcal{A}_k - \mathcal{A}_{k+1}$ . Then

$$\tau(\varphi)(y_i) = [y_i, \bar{w}_i]$$

(where  $\bar{w}_i$  is the class of  $w_i$  in  $\Gamma_k/\Gamma_{k+1}$ ), so the Johnson morphism sends  $\mathcal{L}(hP\Sigma_n \cap \mathcal{A}_*(\text{RF}_n))$  into  $\text{Der}_\tau$ . Moreover, it is injective by Theorem 2.4, and since  $\tau(\chi_{ij}) = d_{ij}$ , Proposition 2.7 implies that it is surjective. □

Theorem 2.9, together with Proposition 2.7, have an interesting consequence: the group  $hP\Sigma_n$  is maximal among subgroups of  $\text{Aut}(\text{RF}_n)$  for which the Andreadakis equality can be true. Indeed, let  $hP\Sigma_n \subsetneq G \subseteq \text{Aut}(\text{RF}_n)$ , and consider the comparison morphism  $i_*: \mathcal{L}(G) \rightarrow \mathcal{L}(G \cap \mathcal{A}_*)$  obtained from the inclusion of  $\Gamma_*G$  into  $G \cap \mathcal{A}_*$ . On the one hand, the Lie algebra  $\mathcal{L}(G \cap \mathcal{A}_*)$  contains  $\mathcal{L}(hP\Sigma_n \cap \mathcal{A}_*)$ , and this inclusion must be strict, otherwise we could argue as in the proof of Lemma 5.3 to show that  $G = hP\Sigma_n$ . On the other hand,  $\mathcal{L}(G)$  is generated in degree 1, so that  $i_*(\mathcal{L}(G)) \subseteq \mathcal{L}(hP\Sigma_n \cap \mathcal{A}_*)$ , the latter being the subalgebra of  $\mathcal{L}(\mathcal{A}_*(\text{RF}_n)) \cong \text{Der}(R\mathcal{L}_n)$  generated by its degree one. As a consequence,  $i_*$  cannot be surjective, whence the conclusion.

Here is another consequence of these theorems:

**Corollary 2.10** The group  $hP\Sigma_n$  is generated by the  $\chi_{ij}$  ( $i \neq j$ ), and  $hP\Sigma_n^{\text{ab}}$  identifies with the free abelian group generated by the  $\bar{\chi}_{ij}$ .

In particular, the canonical morphism from  $P\Sigma_n$  to  $hP\Sigma_n$  is surjective. This means that when it comes to basis-conjugating automorphisms, all automorphisms of  $\text{RF}_n$  are tame. This is in striking contrast with the case of free nilpotent groups [Darné 2019, Section 2.6]. This fact is in fact obvious from the geometrical interpretation (recalled in Section 4), but we give an algebraic proof here, using much less machinery.

**Proof of Corollary 2.10** Thanks to Proposition 2.7 and Theorem 2.9, we know that the classes of the  $\chi_{ij}$  in  $\mathcal{L}(\mathcal{A}_* \cap hP\Sigma_n)$  generate this Lie ring. By applying Lemma 5.3 to the finite filtration  $\mathcal{A}_* \cap hP\Sigma_n$ , we deduce that the  $\chi_{ij}$  generate  $hP\Sigma_n$ .

As a consequence, the  $\bar{\chi}_{ij}$  generate its abelianization. Moreover, the Johnson morphism from  $hP\Sigma_n^{\text{ab}}$  to  $\text{Der}_1(R\mathcal{L}_n)$  sends the  $\bar{\chi}_{ij}$  to the linearly independent elements  $d_{ij}$  of  $\text{Der}_1(R\mathcal{L}_n)$ . Thus the  $\bar{\chi}_{ij}$  are a basis of  $hP\Sigma_n^{\text{ab}}$ . □

We can also use the proof of Proposition 2.7 to compute the Hirsch rank of the nilpotent group  $hP\Sigma_n$  (which is the rank of any associated Lie algebra). We recover the formula of [Audoux et al. 2017b, Remark 4.9]:

**Corollary 2.11** *The Hirsch rank of the reduced McCool group is*

$$\text{rk}(hP\Sigma_n) = \text{rk}(\text{Der}_\tau(R\mathcal{L}_n)) = n \cdot \text{rk}(R\mathcal{L}_{n-1}) = \sum_{k=1}^{n-1} \frac{n!}{(n-k-1)! \cdot k}.$$

**Proof** The first equality is a direct consequence of Theorem 2.9. The second one stems from the proof of Proposition 2.7, where we have shown that  $\text{Der}_\tau(R\mathcal{L}_n)$  is (linearly) a direct sum of  $n$  copies  $D_i$  of  $R\mathcal{L}_{n-1}$ . The last one is a direct application of Proposition 1.9. □

### 3 The Andreadakis problem

The McCool group  $P\Sigma_n \subset \text{Aut}(F_n)$  is generated by the elements  $\chi_{ij} : x_i \mapsto x_i^{x_j}$  ( $\chi_{ij}$  fixes all the other  $x_t$ ). The following relations, called the *McCool relations*, are known to define a presentation of the McCool group  $P\Sigma_n$  [1986]. The reader can easily check that they are satisfied in  $P\Sigma_n$ :

$$\begin{aligned} [\chi_{ik}\chi_{jk}, \chi_{ij}] &= 1 && \text{for } i, j, k \text{ pairwise distinct,} \\ [\chi_{ik}, \chi_{jk}] &= 1 && \text{for } i, j, k \text{ pairwise distinct,} \\ [\chi_{ij}, \chi_{kl}] &= 1 && \text{if } \{i, j\} \cap \{k, l\} = \emptyset. \end{aligned}$$

Thanks to Corollary 2.10, we know that  $hP\Sigma_n$  is naturally a quotient of  $P\Sigma_n$ . We will give in Section 5 three families of relations that need to be added to a presentation of  $P\Sigma_n$  in order to get a presentation of  $hP\Sigma_n$ . This will rely on the semidirect product decomposition that we now describe.

#### 3.1 A semidirect product decomposition

The following decomposition theorem is the central result of the present paper. From it we will deduce the Andreadakis equality for  $hP\Sigma_n$  (Section 3.3) and a presentation of this group and of its Lie ring (Section 5):

**Theorem 3.1** *There is a decomposition of  $hP\Sigma_n$  as a semidirect product,*

$$hP\Sigma_n \cong \left[ \left( \prod_{i < n} \mathcal{N}(x_n)/x_i \right) \rtimes (\mathbf{RF}_n/x_n) \right] \rtimes hP\Sigma_{n-1},$$

where  $\mathcal{N}(x_n)/x_i$  is the normal closure of  $x_n$  inside  $\mathbf{RF}_n/x_i$ , and the action of  $\mathbf{RF}_n/x_n \cong \mathbf{RF}_{n-1}$  on the product is the diagonal one. Moreover, the semidirect product on the right is an almost direct one.

We prove this theorem in three steps. First, we show that  $hP\Sigma_n$  decomposes into a semidirect product  $\mathcal{K}_n \rtimes hP\Sigma_{n-1}$ . Then we investigate the structure of  $\mathcal{K}_n$ , which decomposes as  $\mathcal{K}'_n \rtimes \mathbf{RF}_{n-1}$ . Finally, we investigate the structure of  $\mathcal{K}'_n$ , which is abelian and decomposes as the direct product of the  $\mathcal{N}(x_n)/x_i$ .

**Step 1: decomposition of  $hP\Sigma_n$**  Elements of  $hP\Sigma_n$  preserve the conjugacy class of  $x_n$ , so they preserve its normal closure  $\mathcal{N}(x_n)$ . As a consequence, any of these automorphisms induces a well-defined automorphism of  $\mathbf{RF}_n/\mathcal{N}(x_n) \cong \mathbf{RF}_{n-1}$ . In other words, the projection  $x_n \mapsto 1$  from  $\mathbf{RF}_n$  onto  $\mathbf{RF}_{n-1}$  induces a well-defined morphism  $p_n$  from  $hP\Sigma_n$  to  $hP\Sigma_{n-1}$ . Moreover, this morphism is a split projection, a splitting  $s_n$  being the map extending automorphisms by making them fix  $x_n$ . Let us denote by  $\mathcal{K}_n$  the kernel of  $p_n$ . We thus get our first decomposition,

$$(3-1) \quad hP\Sigma_n \cong \mathcal{K}_n \rtimes hP\Sigma_{n-1}.$$

Moreover, it will follow from [Lemma 3.3](#) below that this is indeed an almost direct product:  $\mathcal{K}_n^{\text{ab}}$  is generated by the classes of the  $\chi_{in}$  and the  $\chi_{ni}$ . From [Corollary 2.10](#), we know that these are sent to linearly independent elements in  $hP\Sigma_n^{\text{ab}}$ , so they freely generate  $\mathcal{K}_n^{\text{ab}}$ . We thus get a direct product decomposition  $hP\Sigma_n^{\text{ab}} \cong \mathcal{K}_n^{\text{ab}} \oplus hP\Sigma_{n-1}^{\text{ab}}$ , as announced.

**Step 2: structure of  $\mathcal{K}_n$**  We first state an easy result on generators of factors in semidirect products.

**Lemma 3.2** *Let  $G = H \rtimes K$  be a semidirect product of groups. Suppose we are given a family  $(h_i)$  of elements of  $H$ , and a family  $(k_j)$  of elements of  $K$  such that their reunion generates  $G$ . Then  $K$  is generated by the  $k_j$ , and  $H$  is generated by the  $h_i^k$ , for  $k \in K$ .*

**Proof** Take an element  $g \in G$  and write it as a product of  $h_i^{\pm 1}$  and  $k_j^{\pm 1}$ . Then use the formula  $kh = ({}^k h)k$  to push the  $k_j$  to the right. We obtain a decomposition  $g = h'k$ , where  $h' \in H$  is a product of conjugates of the  $h_i^{\pm 1}$  by elements of  $K$ , and  $k \in K$  is a product of the  $k_j^{\pm 1}$ . This decomposition has to be the unique decomposition of  $g$  into a product of an element of  $H$  followed by and element of  $K$ . As a consequence, if  $g \in H$ , then  $g = h'$ , whereas if  $g \in K$ , then  $g = k$ , proving our claim. □

We can apply [Lemma 3.2](#) to the  $\chi_{ij}$  in  $hP\Sigma_n \cong \mathcal{K}_n \rtimes hP\Sigma_{n-1}$ . Indeed, the  $\chi_{in}$  and the  $\chi_{ni}$  are in  $\mathcal{K}_n$ , and the other  $\chi_{ij}$  belong to  $hP\Sigma_{n-1}$ . Hence,  $\mathcal{K}_n$  is generated by the conjugates of the  $\chi_{in}$  and the  $\chi_{ni}$  by products of the other  $\chi_{ij}$  and their inverses. In fact, more is true:

**Lemma 3.3** *The group  $\mathcal{K}_n$  is generated by the  $\chi_{in}$  and the  $\chi_{ni}$ .*

**Proof** We use the above relations to show that the subgroup  $H$  of  $\mathcal{K}_n$  generated by the  $\chi_{in}$  and the  $\chi_{ni}$  is normal in  $hP\Sigma_n$ , that is,  $[hP\Sigma_n, H] \subseteq H$ .

The commutator  $[\chi_{in}, \chi_{\alpha\beta}]$  is obviously in  $H$  if  $\alpha = n$  or  $\beta = n$ . Otherwise, it is trivial, except possibly when  $\alpha = i$  or  $\beta = i$ . In the first case (since  $\chi_{n\beta}$  and  $\chi_{i\beta}$  commute),

$$1 = [\chi_{in}, \chi_{n\beta}\chi_{i\beta}] = [\chi_{in}, \chi_{n\beta}]^{(\chi_{n\beta}[\chi_{in}, \chi_{i\beta}])},$$

whence  $[\chi_{in}, \chi_{i\beta}] \in H$ . In the second case,

$$1 = [\chi_{in}\chi_{\alpha n}, \chi_{\alpha i}] = (\chi_{in}[\chi_{\alpha n}, \chi_{\alpha i}])([\chi_{in}, \chi_{\alpha i}]},$$

so, using the first case,  $[\chi_{in}, \chi_{\alpha i}] \in H$ .

In a similar fashion, the bracket  $[\chi_{ni}, \chi_{\alpha\beta}]$  belongs to  $G$  if  $\alpha = n$  or  $\beta = n$ . Otherwise, it is trivial, except when  $\alpha = i$ . But in this case,

$$1 = [\chi_{ni}, \chi_{i\beta}\chi_{n\beta}] = [\chi_{ni}, \chi_{i\beta}]^{(\chi_{n\beta}[\chi_{in}, \chi_{n\beta}])},$$

so  $[\chi_{ni}, \chi_{i\beta}] \in H$ . Thus,  $H$  is stable under conjugation by all generators of  $hP\Sigma_n$ , so it is normal in  $hP\Sigma_n$ . □

**Remark 3.4** We have used only the McCool relations here, so the analogue of [Lemma 3.3](#) is also true in  $P\Sigma_n$ .

By looking at how elements of  $\mathcal{K}_n$  act on  $x_n$ , we get a split projection  $q_n$  from  $\mathcal{K}_n$  onto  $\text{RF}_{n-1}$ . Namely, if  $\varphi \in \mathcal{K}_n$  is an automorphism sending each  $x_i$  to  $x_i^{w_i}$ ,  $q_n$  sends  $\varphi$  onto the class  $\bar{w}_n \in \text{RF}_n/x_n \cong \text{RF}_{n-1}$ . This is well defined, because of [Lemma 1.17](#),

$$x_n^v = x_n^w \iff x_n^{vw^{-1}} = 1 \iff vw^{-1} \in C(x_n) = \mathcal{N}(x_n) \iff \bar{v} = \bar{w}.$$

Moreover, this defines a morphism. Indeed, if  $\varphi$  and  $\psi$  send  $x_n$  respectively to  $x_n^{w_n}$  and  $x_n^{v_n}$ , then

$$\psi\varphi(x_n) = \psi(x_n^{w_n}) = x_n^{v_n\psi(w_n)},$$

and since  $\psi \in \mathcal{K}_n$ , we have  $\overline{\psi(w_n)} = \bar{w}_n$ , whence

$$q_n(\psi\varphi) = \overline{v_n\psi(w_n)} = \bar{v}_n\bar{w}_n = q_n(\psi)q_n(\varphi).$$

This morphism  $q_n$  is a retraction of the inclusion  $t_n$  of  $\text{RF}_{n-1} \cong \text{RF}_n/x_n$  into  $\mathcal{K}_n$  sending  $w \in \text{RF}_n$  to the automorphism fixing all  $x_i$  save  $x_n$ , which is sent to  $x_n^w$ . If we call  $\mathcal{K}'_n$  the kernel of  $q_n$ , we thus get a decomposition

$$(3-2) \quad \mathcal{K}_n = \mathcal{K}'_n \rtimes \text{RF}_{n-1}.$$

**Lemma 3.5** *The above decomposition is  $hP\Sigma_{n-1}$ -equivariant, with respect to the action of  $hP\Sigma_{n-1}$  on  $\mathcal{K}_n$  (and on  $\mathcal{K}'_n \subset \mathcal{K}_n$ ) coming from conjugation in  $hP\Sigma_n$ , and to the canonical action of  $hP\Sigma_{n-1}$  on  $\text{RF}_{n-1}$ . Precisely,  $q_n$  and  $t_n$  are  $hP\Sigma_{n-1}$ -equivariant morphisms.*

**Proof** If  $\varphi \in \mathcal{K}_n$  sends  $x_i$  to  $x_i^{w_i}$  as above, and  $\chi \in hP\Sigma_{n-1}$ , then  $\chi\varphi\chi^{-1}$  sends  $x_n$  to  $x_n^{\chi(w_n)}$ , so

$$q_n(\chi\varphi\chi^{-1}) = \overline{\chi(w_n)} = \chi(\bar{w}_n) = \chi(q_n(\varphi)).$$

As for the equivariance of  $t_n$ , if  $w \in \text{RF}_{n-1}$ , both  $\chi \cdot t_n(w) \cdot \chi^{-1}$  and  $t_n(\chi(w))$  fix all  $x_i$  save  $x_n$ , the latter being sent to  $x_n^{\chi(w)}$ , hence they are equal. □

**Remark 3.6** A similar decomposition holds in  $P\Sigma_n$ , replacing  $\text{RF}_{n-1}$  by  $F_{n-1}$ . The same proof works, replacing the equality  $C(x_n) = \mathcal{N}(x_n)$  (which is not true in this case) by the inclusion  $C(x_n) \subset \mathcal{N}(x_n)$ .

**Step 3: structure of  $\mathcal{K}'_n$**  So far, we have not really used the fact that we consider welded braids up to homotopy (that is, automorphisms of  $\text{RF}_n$ , not of  $F_n$ ). In fact, the analogues of the decomposition results above are true in the group  $P\Sigma_n$  of welded braids (see Remarks 3.4 and 3.6). We now come to the part where the homotopy relation plays a crucial role. That is, we are going to use the relations defining  $\text{RF}_n$  in a crucial way. These relations, saying that each element  $x_i$  of the fixed basis commutes with its conjugates, can be rewritten as

$$\forall i \leq n \quad \forall s, t \in \text{RF}_n \quad x_i^{s x_i t} = x_i^{s t}.$$

In other words, for  $w \in \text{RF}_n$ ,  $x_i^w$  depends only on the class of  $w$  modulo  $x_i$  (that is, modulo the normal closure of  $x_i$ ). These relations allow us to say more about the above decomposition of  $\mathcal{K}_n$ :

**Lemma 3.7** *The kernel  $\mathcal{K}'_n$  of the projection  $q_n: \mathcal{K}_n \twoheadrightarrow \text{RF}_{n-1}$  is an abelian group, isomorphic to the product of the  $\mathcal{N}(x_n)/x_i$ , where  $\mathcal{N}(x_n)/x_i$  is the normal closure of  $x_n$  inside  $\text{RF}_n/x_i \cong \text{RF}_{n-1}$ . Precisely, the identification of  $\mathcal{N}(x_n)/x_i$  with a factor of  $\mathcal{K}'_n$  is induced by the map*

$$c_i: \mathcal{N}(x_n)/x_i \rightarrow \mathcal{K}'_n, \quad u \mapsto \left( x_j \mapsto \begin{cases} x_i^u & \text{if } j = i \\ x_j & \text{otherwise} \end{cases} \right),$$

which is a well-defined group morphism. Furthermore,  $c_i$  is  $\text{RF}_{n-1}$ -equivariant, where  $\text{RF}_{n-1} \cong \langle \chi_{nj} \rangle_j$  acts via automorphisms on the source, and via conjugation on the target.

**Proof** We identify elements  $w \in \text{RF}_{n-1}$  with their image by  $t_n: \text{RF}_{n-1} \rightarrow \mathcal{K}_n$ , that is, we denote by  $w$  the automorphism fixing all  $x_i$  save  $x_n$ , which is sent to  $x_n^w$ . Applying Lemma 3.2 to the semidirect product decomposition (3-2), we see that  $\mathcal{K}'_n$  is generated by the elements  $\chi_{in}^w$ , which we now compute. The automorphism  $\chi_{in}^w$  fixes  $x_\alpha$  if  $\alpha \notin \{i, n\}$ . On  $x_i$  and  $x_n$ , using that  $\chi_{in}(w) \equiv w \pmod{x_n}$ , we compute

$$\chi_{in}^w: x_i \mapsto x_i \mapsto x_i^{x_n} \mapsto x_i^{x_n^w}, \quad \chi_{in}^w: x_n \mapsto x_n \mapsto x_n^w \mapsto \chi_{in}(w)x_n = x_n^w \mapsto x_n.$$

From this calculation, we see that all  $\chi = \chi_{in}^w$  commute with every  $\chi' = \chi_{jn}^v$ , showing that  $\mathcal{K}'_n$  is indeed abelian. If  $j \neq i$ , this is a consequence of the fact that these automorphisms act trivially modulo  $x_n$ ,

$$\chi'(x_i^{x_n^w}) = x_i^{x_n^{\chi'(w)}} = x_i^{x_n^w}.$$

For  $i = j$ , it follows from the fact that the conjugates of  $x_n$  commute.

Consider now  $N_i$  the subgroup generated by the  $\chi_{i_n}^w$ , for  $w \in \text{RF}_{n-1}$ . The elements of  $N_i$  are automorphisms fixing all  $x_j$  save  $x_i$ , and sending  $x_i$  to an element  $x_i^u$ , for some  $u \in \mathcal{N}(x_n)$ . As a consequence, the map  $c_i$  is a surjection from  $\mathcal{N}(x_n)$  onto  $N_i$ . Since, by definition of the reduced free group,  $x_i^{s x_i t} = x_i^{st}$  for all  $s, t \in \text{RF}_n$ , we see that  $c_i(v)$  depends only on the class  $\bar{v}$  of  $v$  in  $\text{RF}_{n-1}/x_i$ . We use this to show that  $c_i$  is a morphism,

$$c_i(u)c_i(v): x_i \mapsto c_i(u)(x_i^{\bar{v}}) = (x_i^{\bar{u}})^{c_i(u)(\bar{v})} = x_i^{\bar{u}\bar{v}} = c_i(uv)(x_i).$$

Now, the kernel of  $c_i$  is  $C(x_i) \cap \mathcal{N}(x_n) = \mathcal{N}(x_i) \cap \mathcal{N}(x_n)$  (using Lemma 1.17). It thus induces an isomorphism between  $\mathcal{N}(x_n)/(\mathcal{N}(x_i) \cap \mathcal{N}(x_n))$  and  $N_i$ . Moreover, since it is the image of  $\mathcal{N}(x_n)$  in  $\text{RF}_n/\mathcal{N}(x_i)$ , this group identifies with the normal closure of  $x_n$  inside  $\text{RF}_n/x_i \cong \text{RF}_{n-1}$ .

We are left to show that  $c_i$  is  $\text{RF}_{n-1}$ -equivariant. It is enough to show that it commutes with the actions of the generators. If  $\varphi \in \langle \chi_{nj} \rangle_{j \neq i}$ , then  $x_i$  does not appear in  $\varphi(x_n)$ , so

$$c_i(u)^\varphi: x_i \mapsto x_i \mapsto x_i^u \mapsto x_i^{\varphi(u)}, \quad c_i(u)^\varphi: x_n \mapsto \varphi(x_n) \mapsto \varphi(x_n) \mapsto x_n,$$

showing that  $c_i(u)^\varphi = c_i(\varphi(u))$ . It remains to check that  $c_i(u)^{\chi_{ni}} = c_i(\chi_{ni}(u))$ ;  $c_i(\chi_{ni}(u))$  identifies with  $c_i(u)$ , since  $\chi_{ni}$  acts trivially modulo  $x_i$ . We thus need to check that  $\chi_{ni}$  commutes with all the  $c_i(u)$  (which are all elements in  $N_i$ ). This comes from the two relations  $x_n^{x_i} = x_n^{x_i^u}$  (because  $u \in \mathcal{N}(x_n)$ ) and  $x_i^{\chi_{ni}(u)} = x_i^u$  (because  $\chi_{ni}$  acts trivially modulo  $x_i$ ). This finishes the proof of the lemma, and of Theorem 3.1. □

### 3.2 The Lie algebra of the reduced McCool group

The decomposition of  $hP\Sigma_n$  described in Theorem 3.1 induces a decomposition of its Lie algebra:

**Theorem 3.8** *The Lie algebra  $\mathcal{L}(hP\Sigma_n)$  decomposes into a semidirect product,*

$$\mathcal{L}(hP\Sigma_n) \cong \left[ \left( \prod_{i < n} \langle y_i \rangle \right) \rtimes R\mathcal{L}_{n-1} \right] \rtimes \mathcal{L}(hP\Sigma_{n-1}),$$

where  $\langle y_i \rangle$  is the ideal generated by  $y_i$  inside  $R\mathcal{L}_{n-1}$ , and the action of  $R\mathcal{L}_{n-1}$  on the product is the diagonal one.

**Proof** From the almost-direct product decomposition  $hP\Sigma_n \cong \mathcal{H}_n \rtimes hP\Sigma_{n-1}$ , comes a decomposition of the Lie algebra  $\mathcal{L}(hP\Sigma_n) \cong \mathcal{L}(\mathcal{H}_n) \rtimes \mathcal{L}(hP\Sigma_{n-1})$ . In the decomposition of  $\mathcal{H}_n$  described in (3-2), we can replace the normal closure  $\mathcal{N}(x_n)/x_i$  of  $x_n$  in  $\text{RF}_n/x_i$  by the normal closure  $\mathcal{N}(x_i)/x_n$  of  $x_i$  in  $\text{RF}_n/x_n \cong \text{RF}_{n-1}$ . Indeed, the automorphism of  $\text{RF}_n$  exchanging  $x_i$  and  $x_n$  induces an isomorphism between these two, which is  $\text{RF}_{n-1}$ -equivariant, since  $x_i$  acts trivially on both of them. We thus have to compute

$$\mathcal{L}(\mathcal{H}_n) \cong \mathcal{L} \left[ \left( \prod_{i < n} \mathcal{N}(x_i) \right) \rtimes \text{RF}_{n-1} \right].$$



Since this is not a decomposition into an almost direct product, we have to use Section 3.1 of [Darné 2021]: we need to compute  $\Gamma_*^{\text{RF}_{n-1}}(\prod \mathcal{N}(x_i))$ , which is the product  $\prod \Gamma_*^{\text{RF}_{n-1}}(\mathcal{N}(x_i))$ , since  $\text{RF}_{n-1}$  acts diagonally. In order to do this, consider the split short exact sequence of groups,

$$\mathcal{N}(x_i) \hookrightarrow \text{RF}_{n-1} \twoheadrightarrow \text{RF}_{n-1}/x_i \cong \text{RF}_{n-2}.$$

From [Darné 2021, Proposition 3.4], this gives rise to a decomposition of  $\Gamma_*(\text{RF}_{n-1})$  into a semidirect product  $\Gamma_*^{\text{RF}_{n-2}}(\mathcal{N}(x_i)) \rtimes \Gamma_*(\text{RF}_{n-2})$ , where  $\Gamma_*^{\text{RF}_{n-2}}(\mathcal{N}(x_i))$  is defined by taking commutators with  $\mathcal{N}(x_i) \rtimes \text{RF}_{n-2} \cong \text{RF}_{n-1}$  at each step, so is equal to  $\Gamma_*^{\text{RF}_{n-1}}(\mathcal{N}(x_i))$ . As a consequence,  $\mathcal{N}_*(x_i) := \Gamma_*^{\text{RF}_{n-1}}(\mathcal{N}(x_i))$  is the intersection of  $\Gamma_*(\text{RF}_{n-1})$  with  $\mathcal{N}(x_i)$ . Its associated Lie algebra fits into the short exact sequence

$$\mathcal{L}(\mathcal{N}_*(x_i)) \hookrightarrow \mathcal{L}(\text{RF}_{n-1}) \twoheadrightarrow \mathcal{L}(\text{RF}_{n-2}).$$

**Theorem 1.12** ensures that the projection on the right identifies with the projection of  $R\mathcal{L}_{n-1}$  onto  $R\mathcal{L}_{n-2}$  sending  $y_i$  to 0, whose kernel is  $\langle y_i \rangle$ . Thus  $\mathcal{L}(\mathcal{N}_*(x_i)) \cong \langle y_i \rangle$ , and

$$\mathcal{L}(\mathcal{N}(x_i) \rtimes \text{RF}_{n-1}) \cong \mathcal{L}(\mathcal{N}_*(x_i)) \rtimes \mathcal{L}(\text{RF}_{n-1}) \cong \langle y_i \rangle \rtimes R\mathcal{L}_{n-1}. \quad \square$$

### 3.3 The Andreadakis equality

**Theorem 3.8** gives a complete description of the graded Lie ring associated to  $\Gamma_*(hP\Sigma_n)$ . On the other hand, **Theorem 2.9** describes the Lie ring associated with the Andreadakis filtration  $hP\Sigma_n \cap \mathcal{A}_*(\text{RF}_n)$ . Using these two results, we are now able to show:

**Theorem 3.9** *The Andreadakis equality holds for  $hP\Sigma_n$ .*

**Proof** We want to show that the Johnson morphism  $\tau' : \mathcal{L}(hP\Sigma_n) \rightarrow \text{Der}(R\mathcal{L}_n)$  is injective (see the end of **Section 0.1**). We make use of the commutative diagram

$$\begin{array}{ccccc} \mathcal{L}(\mathcal{H}_n) & \hookrightarrow & \mathcal{L}(hP\Sigma_n) & \twoheadrightarrow & \mathcal{L}(hP\Sigma_{n-1}) \\ \downarrow \tau' & & \downarrow \tau' & & \downarrow \tau' \\ \bullet & \hookrightarrow & \text{Der}_\tau(R\mathcal{L}_n) & \twoheadrightarrow & \text{Der}_\tau(R\mathcal{L}_{n-1}) \end{array}$$

where the bottom projection is the one induced by  $y_n \mapsto 0$ . By induction (beginning at  $n = 2$ ), using the snake lemma, we only have to prove that the left map is injective, that is, that  $\tau' : \mathcal{L}(\mathcal{H}_n) \rightarrow \text{Der}(R\mathcal{L}_n)$  is. Take an element

$$\varphi = ((w_i), w_n) \in \Gamma_j(\mathcal{H}_n) = \left( \prod_{j < n} (\Gamma_j(\text{RF}_n) \cap \mathcal{N}(x_n)) / x_i \right) \rtimes \Gamma_j(\text{RF}_{n-1}),$$

meaning that  $\varphi$  is the automorphism conjugating  $x_n$  by  $w_n \in \Gamma_j(\text{RF}_{n-1})$  and  $x_i$  by  $w_i \in \Gamma_j(\text{RF}_n) \cap \mathcal{N}(x_n)$  for  $i < n$ , which depends only on the class of each  $w_i$  modulo  $\mathcal{N}(x_i)$ . Then  $\tau'_j(\bar{\varphi})$  sends each  $y_i$  ( $i \leq n$ ) to  $[y_i, \bar{w}_i] \in \mathcal{L}_{j+1}(\text{RF}_n)$ . As a consequence, the equality  $\tau'_j(\bar{\varphi}) = 0$  would mean that each  $\bar{w}_i$  commutes



with  $y_i$  in  $\mathcal{L}(\mathbf{RF}_n) \cong R\mathcal{L}_n$ . By Lemma 1.18, this would imply that  $\bar{w}_i \in \langle y_i \rangle$ . However, in the course of the proof of Theorem 3.8, we have shown that  $\langle y_i \rangle = \mathcal{L}(\Gamma_*(\mathbf{RF}_n) \cap \mathcal{N}(x_i))$ . Thus there exists  $v_i$  in  $\Gamma_j(\mathbf{RF}_n) \cap \mathcal{N}(x_i)$  such that  $\bar{v}_i = \bar{w}_i$ , that is,  $w_i \equiv v_i \pmod{\Gamma_{j+1}(\mathbf{RF}_n)}$ . But we can replace  $w_i$  by  $w_i v_i^{-1}$  without changing  $\varphi$ , so all the  $w_i$  can be chosen to be in  $\Gamma_{j+1}(\mathbf{RF}_n)$ . This implies that  $\varphi \in \Gamma_{j+1}(hP\Sigma_n)$ , which means that  $\bar{\varphi} = 0$  in  $\mathcal{L}_j(hP\Sigma_n)$ . This ends the proof that the kernel of  $\tau'$  is trivial, and the proof of the theorem.  $\square$

### 3.4 Braids up to homotopy

Consider the (classical) pure braid group  $P_n$ . It can be embedded into the monoid of string-links on  $n$  strands. These string-links can be considered up to (link-)homotopy, which means that one adds to the isotopy relation the possibility for each strand to cross itself. This relation is obviously compatible with the monoid structure, and since every string-link is in fact homotopic to a braid, this quotient is a quotient of the pure braid group, called the group of braids up to homotopy, denoted by  $hP_n$ .

**3.4.1 Decomposition and Lie algebra** Goldsmith [1974] described  $hP_n$  as a quotient of  $P_n$  by a finite set of relations. These relations say exactly that for  $j < k$ , the generators  $A_{jk}$  commute with their conjugates by elements of  $\langle A_{ik} \rangle_{i < k} \cong F_{k-1}$ . This means exactly that the free factors in the decomposition of  $P_n$  are replaced by reduced free groups,

$$hP_{n+1} \cong \mathbf{RF}_n \rtimes hP_n.$$

This decomposition first appeared explicitly in [Habegger and Lin 1990], where a more topological proof is described.

Such a decomposition is compatible with the decomposition of the (classical) pure braid group, which means that the canonical projections give a morphism of semidirect products:

$$(3-3) \quad \begin{array}{ccccc} F_n & \hookrightarrow & P_{n+1} & \twoheadrightarrow & P_n \\ \downarrow & & \downarrow & & \downarrow \\ \mathbf{RF}_n & \hookrightarrow & hP_{n+1} & \twoheadrightarrow & hP_n \end{array}$$

(Note: Curved arrows in the original image indicate a commutative diagram structure between the top and bottom rows.)

Since Goldsmith’s relations are commutation relations, the projection from  $P_{n+1}$  onto  $hP_{n+1}$  induces an isomorphism between  $P_{n+1}^{\text{ab}}$  onto  $hP_{n+1}^{\text{ab}}$ . As a consequence, since the decomposition  $P_{n+1} \cong F_n \rtimes P_n$  is an almost-direct product decomposition, the decomposition  $hP_{n+1} \cong \mathbf{RF}_n \rtimes hP_n$  also is. It then induces a decomposition of the lower central series and of the corresponding Lie ring. Precisely, we get iterated semidirect product decompositions,

$$(3-4) \quad \Gamma_j(hP_{n+1}) = \Gamma_j(\mathbf{RF}_n) \rtimes \Gamma_j(hP_n),$$

inducing such decompositions of the associated graded Lie rings. Thus we get:

**Proposition 3.10** *The group  $hP_{n+1}$  is  $n$ -nilpotent, and its Lie algebra decomposes as an iterated semidirect product of reduced free Lie algebras,*

$$\mathcal{L}(hP_{n+1}) \cong \mathcal{L}(\mathbf{RF}_n) \rtimes \mathcal{L}(hP_n) \cong R\mathcal{L}_n \rtimes \mathcal{L}(hP_n).$$

From this, we can deduce the Hirsch rank of  $hP_n$ , recovering Milnor’s formula, as quoted in [Habegger and Lin 1990, Section 3]:

**Corollary 3.11** *The group  $hP_n$  has no torsion and its Hirsch rank is*

$$\text{rk}(hP_n) = \sum_{k=1}^{n-1} (k-1)! \binom{n}{k+1}.$$

**Proof** That it has no torsion (even no torsion in its lower central series) comes from the fact that the  $R\mathcal{L}[m]$  do not, according to Proposition 1.9. The same proposition gives us the ranks of the  $R\mathcal{L}[m]_k$ , allowing us to compute

$$\text{rk}(\mathcal{L}_k(hP_n)) = \sum_{m=1}^{n-1} \text{rk}(R\mathcal{L}[m]_k) = (k-1)! \sum_{m=1}^{n-1} \binom{m}{k} = (k-1)! \binom{n}{k+1},$$

the last equality being obtained by iterating Pascal’s formula, or by a combinatorial proof (replacing the choice of  $k$  elements  $t_1, \dots, t_k$  among  $m$  elements, with  $m$  ranging from  $k$  to  $n-1$ , by the choice of  $k+1$  elements  $t_1, \dots, t_k, m+1$  among  $n$  elements).  $\square$

Let us also mention that we can deduce from the decomposition of  $\mathcal{L}(hP_n)$  described in Proposition 3.10 and from the usual presentation of the pure braid group a presentation of this Lie ring, which is a quotient of the Drinfeld–Kohno Lie ring  $\mathcal{L}(P_n)$  of infinitesimal braids (whose rational version was introduced in [Kohno 1985]).

**Corollary 3.12** *The Lie ring of  $hP_n$  is generated by  $t_{ij}$  ( $1 \leq i, j \leq n$ ), under the Drinfeld–Kohno relations*

$$\begin{aligned} t_{ij} &= t_{ji} \text{ and } t_{ii} = 0 && \text{for all } i, j, \\ [t_{ij}, t_{ik} + t_{kj}] &= 0 && \text{for all } i, j, k, \\ [t_{ij}, t_{kl}] &= 0 && \text{if } \{i, j\} \cap \{k, l\} = \emptyset, \end{aligned}$$

to which are added, for each  $m$ , the vanishing of Lie monomials in the  $t_{im}$  ( $i < m$ ) with repetition.

**Proof** The proof in the classical case (see for instance the appendix of [Darné 2021]) adapts verbatim, by considering reduced free Lie rings instead of free Lie rings.  $\square$

Notice that as in the definition of the reduced free Lie ring (Definition 1.6—see also Remark 1.8), one can give a simpler finite presentation by considering, for each  $m$ , only linear Lie monomials in the  $t_{im}$  ( $i < m$ ) of length at most  $m$ .

**3.4.2 The Andreadakis problem** The semidirect product  $\text{RF}_n \rtimes hP_n$  described above is the same thing as an action of  $hP_n$  on  $\text{RF}_n$ , also described by a morphism from  $hP_n$  to  $\text{Aut}(\text{RF}_n)$ . This is the *homotopy Artin action*, that we now study, using the fact that it is encoded by conjugation inside  $hP_{n+1} = \text{RF}_n \rtimes hP_n$ .

First, we remark that this action is by basis-conjugating automorphisms. In fact, the compatibility diagram (3-3) gives rise to a commutative diagram

$$\begin{array}{ccc} P_n & \hookrightarrow & \text{Aut}_C(F_n) \\ \downarrow & & \downarrow \\ hP_n & \xrightarrow{a} & \text{Aut}_C(\text{RF}_n) \end{array}$$

where the morphism on the left is surjective by Corollary 2.10. The top map, which is the Artin action, is injective (the action is faithful) and its image is exactly the subgroup of basis-conjugating automorphisms fixing the *boundary element*  $x_1 \cdots x_n$  [Birman 1974, Theorem 1.9]. Habegger and Lin [1990, Theorem 1.7] have shown that the analogous statements are true for  $hP_n$ : the homotopy Artin action induces an isomorphism between  $hP_n$  and the group  $\text{Aut}_C^{\partial}(\text{RF}_n)$  of basis-conjugating automorphisms of  $\text{RF}_n$  preserving the product  $x_1 \cdots x_n$ . Precisely, they show that the latter admits the same decomposition as  $hP_n$ , and that the pieces of these decompositions are identified under the Artin morphism. We recover the faithfulness of the homotopy Artin action as part of our answer to the Andreadakis problem for  $hP_n \subset \text{Aut}_C(\text{RF}_n)$  (see Corollary 3.14 below).

**Theorem 3.13** *The Andreadakis equality holds for the image of the Artin action  $a : hP_n \rightarrow \text{Aut}(\text{RF}_n)$ . Namely,  $\Gamma_*(hP_n) = a^{-1}(\mathcal{A}_*(\text{RF}_n))$ .*

**Proof** We adapt the proof for  $P_n$  given in [Darné 2021]. Let  $w \in hP_n$ , and suppose that  $w$  acts on  $\text{RF}_n$  as an element of  $\mathcal{A}_j$ . We want to show that it belongs to  $\Gamma_j(hP_n)$ . Our hypothesis can be written as

$$[w, \text{RF}_n] \subseteq \Gamma_{j+1}(\text{RF}_n),$$

where the bracket is computed in  $\text{RF}_n \rtimes hP_n$ , which is exactly  $hP_{n+1}$ . Moreover, from the decomposition of the lower central series of  $hP_{n+1}$  described above (Section 3.4.1), we deduce that

$$\Gamma_j(hP_n) = hP_n \cap \Gamma_j(hP_{n+1}),$$

so the conclusion we seek is in fact  $w \in \Gamma_j(hP_{n+1})$ . Let us comb  $w$ : we write

$$w = \beta_n \cdots \beta_2 \in \text{RF}_{n-1} \rtimes (\text{RF}_{n-2} \rtimes (\cdots \rtimes \text{RF}_1)) = hP_n.$$

Again, because of the decomposition of the lower central series of  $hP_n$ , we need to show that each  $\beta_i$  is in  $\Gamma_j(hP_{n+1})$ . In the rest of the proof, we often write  $\Gamma_k$  for  $\Gamma_k(hP_{n+1})$ , its intersection with the subgroups under consideration being their own  $\Gamma_k$ , because of (3-4).

Let us suppose that  $w \notin \Gamma_j(hP_{n+1})$ . Then  $w \in \Gamma_k - \Gamma_{k+1}$  for some  $k < j$ . Let  $i$  be maximal such that  $\beta_i \notin \Gamma_{k+1}$ . On the one hand, the generator  $A_{i,n+1} \in \text{RF}_n$  commutes with every  $\beta_k$  with  $k < i$ ,

so  $[w, A_{i,n+1}] \equiv [\beta_i, A_{i,n+1}] \pmod{\Gamma_{k+2}}$ . Moreover, by hypothesis,  $[w, A_{i,n+1}] \in \Gamma_{j+1} \subseteq \Gamma_{k+2}$ , so  $[\beta_i, A_{i,n+1}] \in \Gamma_{k+2}$ . Since  $\beta_i$  has degree  $k$  and  $A_{i,n+1}$  has degree 1 in the lower central series, this means that  $[\bar{\beta}_i, \bar{A}_{i,n+1}] = 0$  in the Lie algebra. On the other hand,  $\beta_i$  and  $A_{i,n+1}$  belong to another copy of  $\text{RF}_n$  inside  $hP_{n+1}$ , namely  $\langle A_{1,i}, \dots, A_{i-1,i}, A_{i,i+1}, \dots, A_{i,n+1} \rangle$ . We denote this copy by  $\widetilde{\text{RF}}_n$ . We remark that the equality  $\Gamma_*(\widetilde{\text{RF}}_n) = \widetilde{\text{RF}}_n \cap \Gamma_*(hP_{n+1})$  is also true for this copy of  $\text{RF}_n$ , as one sees by switching the strands  $i$  and  $n + 1$  in the reasoning above. But then we can apply [Lemma 1.18](#): since  $\bar{\beta}_i$  commutes with the generator  $\bar{A}_{i,n+1}$  of  $\mathcal{L}(\widetilde{\text{RF}}_n) \cong \mathcal{L}\mathcal{L}_n$ , it must belong to the Lie ideal of  $\mathcal{L}(\widetilde{\text{RF}}_n)$  generated by  $\bar{A}_{i,n+1}$ . But this is impossible: by definition of  $\beta_i$ , the generator  $\bar{A}_{i,n+1}$  cannot appear in  $\bar{\beta}_i$ . We thus get a contradiction, and our conclusion.  $\square$

From this, we can recover the injectivity part of the result of Habegger and Lin:

**Corollary 3.14** [[Habegger and Lin 1990](#), Theorem 1.7] *The homotopy Artin action is faithful.*

**Proof** If  $w \in hP_n$  acts trivially on  $\text{RF}_n$ , then  $a(w) \in \{1\} = \mathcal{A}_n(\text{RF}_n)$ , so  $w \in \Gamma_n(hP_n)$  by [Theorem 3.13](#). But  $\Gamma_n(hP_n) = \{1\}$  ([Proposition 3.10](#)), whence  $w = 1$ .  $\square$

This injectivity of  $a: hP_n \rightarrow hP\Sigma_n = \text{Aut}_{\mathcal{C}}(\text{RF}_n)$  is weaker than our statement, which says that the lower central series are in fact compatible, since they both are the trace of the Andreadakis filtration  $\mathcal{A}_*(\text{RF}_n)$ :

**Corollary 3.15** *For all  $n$ ,  $hP_n \cap \Gamma_*(hP\Sigma_n) = \Gamma_*(hP_n)$ .*

**Proof** Combine [Theorems 3.13](#) and [3.9](#).  $\square$

**Remark 3.16** The rationalization of the Lie ring  $\mathcal{L}(P_n)$  is exactly  $\mathcal{P}^{hsl}$  of [[Bar-Natan 1995](#), Theorem 3], where different diagrammatic descriptions for its enveloping algebra are discussed.

## 4 Topological interpretation

Consider the group  $P_n$  of pure braids. Via the decomposition  $P_{n+1} \cong F_n \rtimes P_n$ , we get an action of  $P_n$  on the free group  $F_n$ , which is the classical *Artin action*. Geometrically, it is best understood as the action of  $P_n$ , which is the *motion group* of  $n$  points in a plane, on the fundamental group of the plane with  $n$  points removed. As mentioned above ([Section 3.4.2](#)), this action is faithful, giving an embedding of  $P_n$  into  $\text{Aut}(F_n)$ , whose image is exactly the subgroup  $\text{Aut}_{\mathcal{C}}^{\partial}(F_n)$  of automorphisms fixing the conjugacy class of each generator  $x_i$ , and preserving the *boundary element*  $x_1 \cdots x_n$  [[Birman 1974](#), Theorem 1.9].

An analogous statement is true for the group  $P\Sigma_n$  of pure *welded braids*. This group is a group of tube-shaped braids in  $\mathbb{R}^4$ , and can also be seen as the (pure) *motion group* of  $n$  unknotted circles in  $\mathbb{R}^3$  (see [[Damiani 2017](#)] on the different definitions on this group). It acts on the fundamental group of  $\mathbb{R}^3$

with  $n$  unknotted circles removed, which is again the free group  $F_n$ . This *Artin action* is again faithful, and its image is exactly the subgroup  $\text{Aut}_C(F_n)$  of automorphisms fixing the conjugacy class of each generator  $x_i$  [Goldsmith 1981].

The same statements are true *up to (link-)homotopy*. These have been recalled for braids in Section 3.4. For welded braids, link-homotopy of string links also makes sense (in  $\mathbb{R}^4$ ), and for welded diagrams (which are another point of view on these objects), this relation corresponds to virtualization of self-crossings. It has been shown in [Audoux et al. 2017a, Theorem 2.34] that the group of welded braids up to homotopy is isomorphic to the group  $\text{Aut}_C(\text{RF}_n) = hP\Sigma_n$  of automorphisms of  $\text{RF}_n$  fixing the conjugacy class of each generator  $x_i$ .

We sum up the situation with the following diagrams:

$$\begin{array}{ccc}
 & \text{up to isotopy} & \text{up to homotopy} \\
 (4-1) \quad & P_n \xrightarrow{\cong} \text{Aut}_C^\partial(F_n) & hP_n \xrightarrow{\cong} \text{Aut}_C^\partial(\text{RF}_n) \\
 & \downarrow & \downarrow \\
 & P\Sigma_n \xrightarrow{\cong} \text{Aut}_C(F_n) & hP\Sigma_n \xrightarrow{\cong} \text{Aut}_C(\text{RF}_n)
 \end{array}$$

### 4.1 Milnor invariants

Here we interpret our work in terms of *Milnor invariants* of welded braids up to homotopy. Milnor invariants were first defined in [Milnor 1957] for links, as integers with some indeterminacy. It appeared later that they were more naturally defined for string links, for which they are proper integers, the indeterminacy previously observed corresponding exactly to a choice of presentation of a link as the closure of a string-link. Here we focus on their definition for braids, which is not a restrictive choice when working up to homotopy.

If  $\beta$  is a pure braid, we can look at its image via the Artin action, which is a basis-conjugating automorphism  $x_i \mapsto x_i^{w_i}$ . The element  $w_i$  is well defined up to left multiplication by  $x_i^{\pm 1}$ , so it is well defined if we suppose that  $x_i$  does not appear in the class  $\bar{w}_i \in F_n^{\text{ab}}$ . For each  $i$ , one can look at the image of the element  $w_i \in F_n$  by the *Magnus expansion*  $\mu: F_n \hookrightarrow \widehat{T[n]}$ , getting an element of the completion of the free associative ring  $\widehat{T[n]}$  on  $n$  generators  $X_1, \dots, X_n$ , which can be seen as the ring of noncommutative power series on these generators. Recall that the Magnus expansion is defined by  $x_i \mapsto 1 + X_i$ , and it is an injection of the free group  $F_n$  into  $\widehat{T[n]}^\times$ . Then the *Milnor invariants* are the coefficients of the  $\mu(w_i)$ . Precisely, if  $i \leq n$  is an integer, and  $I = (i_1, \dots, i_d)$  is any list of positive integers, then  $\mu_{I,i}(\beta)$  is the coefficient of the monomial  $X_{i_1} \cdots X_{i_d}$  in  $\mu(w_i)$ . Moreover, we call  $d$  the *degree* of the Milnor invariant  $\mu_{I,i}$ .

The first nontrivial Milnor invariants of  $\beta$  can also be obtained through the Johnson morphism. Namely, let  $d$  be the greatest integer such that  $\beta \in \mathcal{A}_d(F_n)$  (we identify  $\beta$  with its image via the Artin action). By definition of  $w_i$ ,  $x_i$  does not appear in the class  $\bar{w}_i \in F_n^{\text{ab}}$ . Thus, we deduce from [Darné 2021,

Lemma 6.3] that for all  $j \geq 1$ ,  $[x_i, w_i] \in \Gamma_{j+1}(F_n)$  if and only if  $w_i \in \Gamma_d(F_n)$ . This implies that  $d$  is maximal such that all  $w_i$  belong to  $\Gamma_j(F_n)$ . The image of  $\bar{\beta} \in \mathcal{A}_d/\mathcal{A}_{d+1}$  by the Johnson morphism is the derivation of the free Lie algebra  $\mathfrak{L}[n]$  given by  $x_i \mapsto [x_i, \bar{w}_i]$ , where  $\bar{w}_i \in \Gamma_d/\Gamma_{d+1}(F_n) \cong \mathfrak{L}[n]_d$  is the class of  $w_i$ , possibly trivial (but nontrivial for at least one  $i$ ).

Now, we can consider the element  $\bar{w}_i$  as being inside  $T[n]_d$ , and the inclusion of  $\mathfrak{L}[n]$  into  $T[n]$  is exactly the graded map induced by the Magnus expansion  $\mu$ . Precisely, if we call  $\hat{T}_1^d$  the ideal of  $T[n]$  defined by elements of valuation at least  $d$  (the valuation of a power series being the total degree of its least nontrivial monomial), then  $\Gamma_d(F_n) = \mu^{-1}(1 + \hat{T}_1^d)$ , and the induced map  $\bar{\mu}: \Gamma_d/\Gamma_{d+1}(F_n) \hookrightarrow \hat{T}_1^d/\hat{T}_1^{d+1}$  identifies with the canonical inclusion of  $\mathfrak{L}[n]_d$  into  $T[n]_d$ . As a consequence, the class  $\bar{w}_i$  is the degree- $d$  part of  $\mu(w_i)$ , which has valuation at least  $d$ . We sum this up in the following:

**Proposition 4.1** *The group  $\mathcal{A}_d(F_n) \cap P_n$  is the set of braids with vanishing Milnor invariants of degree at most  $d - 1$ . Moreover, Milnor invariants of degree  $d$  of these braids can be recovered from their image by the Johnson morphism  $\tau: \mathcal{A}_d/\mathcal{A}_{d+1} \hookrightarrow \text{Der}_d(\mathfrak{L}[n])$ .*

Obviously, since we have not used anywhere that the automorphism  $\beta$  preserves the boundary element, these constructions work for all welded braids (that is, for all basis-conjugating automorphisms of  $F_n$ ).

Let us now explain how to define Milnor invariants for (welded) braids up to homotopy. First, we need to replace  $F_n$  by  $\text{RF}_n$ . Then we can assume that  $x_i$  does not appear in  $w_i$  (since  $x_i^{u x_i v} = x_i^{uv}$  in the reduced free group). The Magnus expansion must be replaced by the morphism (1-1), and we get only Milnor invariants without repetitions (that is,  $I$  must be without repetition in order to define a nontrivial  $\mu_{I,i}$ ). Everything works as described above (using the work done in Section 1.2), so  $\mathcal{A}_d(F_n)$  is exactly the subgroup where invariants of degree at most  $d - 1$  vanish. So we can reformulate Theorems 3.9 and 3.13 as:

**Theorem 4.2** *Homotopy Milnor invariants of degree at most  $d$  classify braids (resp. welded braids) up to homotopy up to elements of  $\Gamma_{d+1}(hP_n)$  (resp.  $\Gamma_{d+1}(hP\Sigma_n)$ ).*

**Remark 4.3** The group  $\Gamma_{d+1}(hP_n)$  can also be seen as the set of braids which are homotopic to elements of  $\Gamma_{d+1}(P_n)$ .

## 4.2 Arrow calculus

We now explain briefly the precise link between our work and the work of Meilhan and Yasuhara [2019]. We will not give any definition here; the reader is referred to their paper for basic definitions and details.

Our understanding of the link between our work and theirs relies on the following remark: *calculus of arrows and  $w$ -trees is the same thing as commutator calculus in the welded braid group  $P\Sigma_n$* . Precisely, when attaching a tree  $T$  to a diagram  $D$ , one has to select the points where the root and leaves of  $T$  are

attached. If we consider a little arc around each of these points, we see that doing so consists of choosing  $n$  strands (which inherit their orientation from  $D$ ). Then the data of  $T$  describes an element of the braid group on these strands, and doing the surgery along  $T$  is exactly the same as inserting the braid described by  $T$  at the chosen spot on  $D$ , to get the new diagram  $D_T$ . Namely, a single arrow from a strand  $j$  to a strand  $i$  describes the insertion of the braid  $\chi_{ij}$ , and a tree with root at  $i$  describes the insertion of a commutator between the  $\chi_{ij}$ , for varying  $j$  (note that any number of strands can be added).

In the light of this remark, we can see that many relations they describe correspond to algebraic relations written in the present paper. Also, two diagrams are  $w_k$ -equivalent if and only if they can be obtained from one another by inserting braids in  $\Gamma_k(P_n)$  (for varying  $n$ ). And we can in fact deduce our Andreadakis equality (Theorem 4.2) from their classification theorem of welded string links up to homotopy [Meilhan and Yasuhara 2019, Theorem 9.4]. They fell short of doing so, stating only their weaker Corollary 9.5. In fact, they did not look for the precise identification between trees and commutator calculus described here. They only knew that something of the sort should be true, but were interested in other matters at the time.

## 5 A presentation of the homotopy loop braid group

Goldsmith [1974] gave a presentation of the braid group up to homotopy (see also Section 3.4). She proved that, to a presentation of the pure braid group with generators  $A_{ij}$ , one has to add the family of relations making each  $\langle A_{1k}, \dots, A_{k-1,k} \rangle$  into a reduced free group. The goal of the present section is to give a similar presentation of the loop braid group up to homotopy. The situation here is more intricate; to a presentation of  $P\Sigma_n$  with generators  $\chi_{ij}$ , we have to add three families of relations:

- (R1) the relations saying that for all  $m$ ,  $\langle \chi_{mk} \rangle_{k < m}$  is reduced;
- (R2)  $[\chi_{im}, w, \chi_{jm}] = 1$ , for  $i, j < m$  and  $w \in \langle \chi_{mk} \rangle_{k < m}$ ;
- (R3)  $[\chi_{im}, w, \chi_{mi}] = 1$ , for  $i < m$  and  $w \in \langle \chi_{mk} \rangle_{k < m, k \neq i}$ .

We remark that because of the symmetry with respect to the generators of  $\text{RF}_n$ , these relations are still true if we replace each symbol “ $<$ ” by a symbol “ $\neq$ ”, which would give a more symmetric (but bigger) set of relations.

**Remark 5.1** These relations also describe the quotient of the group  $wB_n$  of all welded braids by the homotopy relation. Indeed, performing a homotopy cannot move endpoints of string links, so the subgroup of relations must be a subgroup of the *pure* welded braid group, like in the classical setting [Goldsmith 1974, Lemma 1].

### 5.1 Generators of nilpotent groups

One key argument in the determination of a presentation of  $hP\Sigma_n$  consists in lifting generators from Lie rings to groups. Such generators will be obtained from combinatorics in the free Lie ring (see the appendix), and lifting them will use the nilpotence of the groups involved.



**Convention 5.2** By a *finite* filtration, we always mean a separating one; a strongly central series  $G_*$  is *finite* if there exists a  $i \geq 1$  such that  $G_i = \{1\}$ . In particular, if there exists a finite strongly central series on  $G$ , then  $G$  must be nilpotent (recall that  $G_i \supseteq \Gamma_i G$ ).

**Lemma 5.3** Let  $G_*$  be a finite strongly central filtration on a (nilpotent) group  $G$ . Suppose that the  $x_\alpha$  are elements of  $G$  such that their classes  $\bar{x}_\alpha$  generate the Lie ring  $\mathcal{L}(G_*)$ . Then the  $x_\alpha$  generate  $G$ .

**Proof** Consider the subgroup  $K$  of  $G$  generated by the  $x_\alpha$ . The canonical morphism from  $\mathcal{L}(G_* \cap K)$  to  $\mathcal{L}(G_*)$  comes from an injection between filtrations, so it is injective. By hypothesis, it is also surjective. By induction (using the five lemma), we deduce that  $K/(G_j \cap K) = G/G_j$ , for all  $j$ . Since there exists  $j$  such that  $G_j = \{1\}$ , this proves that  $K = G$ .  $\square$

The definition of the Lyndon monomials  $P_w$  (Section A.2) makes sense in any group, if we interpret letters as elements of the group, and brackets as commutators.

**Proposition 5.4** Let  $G$  be a nilpotent group generated by a set  $X$ , and  $x \in X$ . Then the normal closure  $\mathcal{N}(x)$  of  $x$  in  $G$  is generated by Lyndon monomials  $P_w$ , for Lyndon words  $w \in X^*$  containing  $x$ .

**Proof** By taking images in  $G$ , it is enough to show this for the free nilpotent group  $F_j[X] := F[X]/\Gamma_{j+1}$ . In this case,  $\mathcal{N}(x)$  is the kernel of the canonical projection from  $F_j[X]$  to  $F_j[X - \{x\}]$ . Setting  $\mathcal{N}_*(x) := \mathcal{N}(x) \cap \Gamma_*(F_j[X])$ , we get a short exact sequence of filtrations translating into a short exact sequence of Lie rings

$$\mathcal{L}(\mathcal{N}_*(x)) \hookrightarrow \mathcal{L}(F_j[X]) \twoheadrightarrow \mathcal{L}(F_j[X - \{x\}]).$$

Since  $\mathcal{L}(F_j[X])$  is the  $j^{\text{th}}$  truncation of the free Lie algebra on  $Y = \bar{X}$ , and the projection is the canonical one (sending  $y = \bar{x}$  to 0), the subring  $\mathcal{L}(\mathcal{N}_*(x))$  identifies with the  $j^{\text{th}}$  truncation of the ideal  $\langle y \rangle$  of  $\mathcal{L}[Y]$ . This ideal is linearly generated by Lyndon Lie monomials on  $Y$  containing  $y$ . Since these are the classes of the corresponding monomials in the group  $F_j[X]$ , Lemma 5.3 gives the desired conclusion.  $\square$

**Corollary 5.5** Let  $X$  be a set, and  $x \in X$ . The normal closure  $\mathcal{N}(x)$  of  $x$  in  $\text{RF}[X]$  is free abelian on the Lyndon monomials  $P_w$ , for Lyndon words without repetition  $w \in X^*$  containing  $x$ .

**Proof** It is enough to show this for  $X$  finite. Then  $\text{RF}[X]$  is nilpotent, and we can apply Proposition 5.4 to show that Lyndon monomials without repetition containing  $x$  generate  $\mathcal{N}(x)$ . Indeed, in  $\text{RF}[X]$ , the only nontrivial Lyndon monomials in elements of  $X$  are those without repetition. Moreover,  $\mathcal{N}(x)$  is abelian, by definition of  $\text{RF}[X]$ . We are thus left with proving that these elements are linearly independent. But any nontrivial linear relation between them would give a nontrivial linear relation between Lyndon monomials without repetition in  $\mathcal{L}(\text{RF}[X])$  (take  $l$  to be the minimal length of the monomials involved, and project the relation into  $\Gamma_l/\Gamma_{l+1}$ ). Such a relation cannot hold (Proposition 1.9), so this proves the corollary.  $\square$



If  $g, g_1, \dots, g_m$  are elements of a group, let us denote by  $\text{Lynd}(g; g_1, \dots, g_m)$  the family of Lyndon monomials  $(P_w)$ , where  $w$  runs through Lyndon words without repetition on the letters  $g, g_1, \dots, g_m$  which contain  $g$ . When considering these sets, we will choose an order on the letters making all  $g_i$  greater than  $g$ . In that case, elements of  $\text{Lynd}(g; g_1, \dots, g_m)$  are of the form  $[[g, P_v], P_w]$ , where neither  $v$  nor  $w$  contains  $g$ . As usual, we denote by  $(g_1, \dots, \hat{g}_i, \dots, g_m)$  the  $(m-1)$ -tuple obtained from  $(g_1, \dots, g_m)$  by removing the  $i^{\text{th}}$  component.

We now use [Corollary 5.5](#) in order to get a basis of the group  $\mathcal{K}'_n$  introduced in [Section 3](#) from the decomposition obtained in [Lemma 3.7](#).

**Lemma 5.6** *A basis of the abelian group  $\mathcal{K}'_n$  is given by*

$$\bigcup_i \text{Lynd}(\chi_{in}; \chi_{n1}, \dots, \hat{\chi}_{ni}, \dots, \chi_{n,n-1}).$$

**Proof** We use notation from the proof of [Lemma 3.7](#). Equivariance of the isomorphism  $c_i$  ensures that  $c_i^{-1}$  sends the set  $\text{Lynd}(\chi_{in}; \chi_{n1}, \dots, \hat{\chi}_{ni}, \dots, \chi_{n,n-1})$  to the set  $\mathcal{B} := \text{Lynd}(x_n; \chi_{n1}, \dots, \hat{\chi}_{ni}, \dots, \chi_{n,n-1})$ , the latter brackets being computed in the semidirect product  $(\mathcal{N}(x_n)/x_i) \rtimes \langle \chi_{nj} \rangle_j$ . If  $v \in \text{RF}_{n-1}$ , we denote by  $\chi_v$  the automorphism of  $\text{RF}_n$  sending  $x_n$  to  $x_n^v$  and fixing all other generators ( $\chi_v$  was denoted by  $t_n(v)$  above). Elements of  $\mathcal{B}$  are of the form  $[[x_n, \chi_v], \chi_w]$ , where  $\chi_v$  and  $\chi_w$  are Lyndon monomials in the  $\chi_{nj}$  ( $j \neq i$ ), which means exactly that  $v$  and  $w$  are Lyndon monomials in the  $x_j$  ( $j \neq i, n$ ), since  $t_n: v \mapsto \chi_v$  is a morphism. Recall that the class of  $\chi_v$  in the Lie algebra  $\mathcal{L}(\mathcal{A}_*(\text{RF}_n))$  acts on the Lie algebra  $R\mathcal{L}_n$  via the tangential derivation  $\tau(\bar{\chi}_v)$  induced by  $[\chi_v, -]$ , sending  $x_n$  to  $[x_n, v]$  and all other  $x_i$  to 0. As a consequence, the class of  $[[x_n, \chi_v], \chi_w]$  in the Lie algebra  $\mathcal{L}(\mathcal{N}_*(x_n)/x_i) \subset R\mathcal{L}_n$  is

$$\tau(\bar{\chi}_w)\tau(\bar{\chi}_v)(x_n) = \tau(\bar{\chi}_w)([v, x_n]) = [v, [w, x_n]] = [[x_n, w], v],$$

since the derivation  $\tau(\bar{\chi}_w)$  vanishes on  $v$ . As a consequence, the family  $\mathcal{B}$  is another lift of the basis of  $\mathcal{L}(\mathcal{N}_*(x_n)/x_i)$  considered above, and the same proof as the proof of [Corollary 5.5](#) (in  $\text{RF}_n/x_i \cong \text{RF}_{n-1}$ ) shows that it is a basis of  $\mathcal{N}(x_n)/x_i$ , whence the result.  $\square$

**Remark 5.7** In the semidirect product  $(\mathcal{N}(x_n)/x_i) \rtimes \langle \chi_{nj} \rangle_j$  which appears in the proof, the group  $\langle \chi_{nj} \rangle_j$  is isomorphic to  $\text{RF}_{n-1}$  but its action is *not* the conjugation action.

## 5.2 The presentation

Let us recall the relations on the  $\chi_{ij}$  that will give a presentation of  $hP\Sigma_n$ :

- (R0) the McCool relations on the  $\chi_{ij}$  (see the introduction);
- (R1)  $[\chi_{mi}, w, \chi_{mi}] = 1$ , for  $i < m$  and  $w \in \langle \chi_{mk} \rangle_{k < m}$ ;
- (R2)  $[\chi_{im}, w, \chi_{jm}] = 1$ , for  $i, j < m$  and  $w \in \langle \chi_{mk} \rangle_{k < m}$ ;
- (R3)  $[\chi_{im}, w, \chi_{mi}] = 1$ , for  $i < m$  and  $w \in \langle \chi_{mk} \rangle_{k < m, k \neq i}$ .

We now show that they indeed give the presentation that we were looking for:

**Theorem 5.8** *The pure loop braid group up to homotopy  $hP\Sigma_n$  is the quotient of  $P\Sigma_n$  by relations (R1), (R2) and (R3). As a consequence, it admits the presentation*

$$hP\Sigma_n \cong \langle \chi_{ij} \ (i \neq j) \mid (R0), (R1), (R2), (R3) \rangle.$$

**Proof** Let  $\mathcal{G}_n$  be the group defined by the presentation of the theorem. The  $\chi_{ij}$  in  $hP\Sigma_n$  satisfy the above relations. As a consequence, there is an obvious morphism  $\pi$  from  $\mathcal{G}_n$  to  $hP\Sigma_n$ . Since the  $\chi_{ij}$  generate  $hP\Sigma_n$  (Corollary 2.10), this morphism is surjective. We need to show that it is an isomorphism. We will do that by showing that  $\mathcal{G}_n$  admits a decomposition similar to that of  $hP\Sigma_n$ , and that the pieces in the two decompositions are isomorphic via  $\pi$ . We do this in three steps, parallel to the proof of Theorem 3.1.

**Step 1** We define a projection  $\tilde{p}_n$  from  $\mathcal{G}_n$  to  $\mathcal{G}_{n-1}$  by sending  $\chi_{ij}$  to  $\chi_{ij}$  if  $n \notin \{i, j\}$ , and  $\chi_{in}$  and  $\chi_{nj}$  to 1. This morphism is well defined (from the presentations), and so is its obvious section  $\tilde{s}_n: \mathcal{G}_{n-1} \hookrightarrow \mathcal{G}_n$ . If we denote by  $\tilde{\mathcal{K}}_n$  the kernel of  $\tilde{p}_n$ , we get a semidirect product decomposition  $\mathcal{G}_n = \tilde{\mathcal{K}}_n \rtimes \mathcal{G}_{n-1}$  that fits in the following diagram:

$$\begin{array}{ccccc} \tilde{\mathcal{K}}_n & \hookrightarrow & \mathcal{G}_n & \xrightarrow{\tilde{p}_n} & \mathcal{G}_{n-1} \\ \downarrow \text{---} & & \downarrow \pi & \xleftarrow{s_n} & \downarrow \pi \\ \mathcal{K}_n & \hookrightarrow & hP\Sigma_n & \xrightarrow{p_n} & hP\Sigma_{n-1} \end{array}$$

By induction (using the five lemma), beginning with the isomorphism  $\mathcal{G}_2 \cong hP\Sigma_2 \cong \mathbb{Z}^2$  (which is the group  $\langle \chi_{12}, \chi_{21} \rangle$  of inner automorphisms of  $RF_2$ ), we only need to show that the induced morphism between the kernels are isomorphisms.

**Step 2** We can apply Lemma 3.2 to the above decomposition of  $\mathcal{G}_n$ ; the proof of Lemma 3.3 only used the McCool relations, so it carries over without change to show that  $\tilde{\mathcal{K}}_n$  is generated by the  $\chi_{in}$  together with the  $\chi_{nj}$ . This shows directly that the map from  $\tilde{\mathcal{K}}_n$  to  $\mathcal{K}_n$  is surjective (this fact also comes from the snake lemma and the induction hypothesis). Consider the map  $\tilde{\mathcal{K}}_n \rightarrow \mathcal{K}_n \twoheadrightarrow RF_n$ , where the second map is the projection  $q_n$  from  $\mathcal{K}_n$  to  $RF_{n-1}$  defined in the proof of Theorem 3.1. This map sends the  $\chi_{in}$  to 1 and the  $\chi_{nj}$  to the  $x_j$ . From the relations (R1), we know that the assignment  $x_j \mapsto \chi_{nj}$  defines a section  $\tilde{t}_n$  from  $RF_{n-1}$  to  $\tilde{\mathcal{K}}_n$ . This shows that the  $\chi_{nj}$  generate a reduced free group inside  $\tilde{\mathcal{K}}_n$ . If we denote by  $\tilde{\mathcal{K}}'_n$  the kernel of  $\tilde{q}_n = q_n \circ \pi$ , we get a semidirect product decomposition  $\tilde{\mathcal{K}}_n = \tilde{\mathcal{K}}'_n \rtimes RF_{n-1}$ , similar to (3-2), that fits in the following diagram:

$$\begin{array}{ccccc} \tilde{\mathcal{K}}'_n & \hookrightarrow & \tilde{\mathcal{K}}_n & \xrightarrow{\tilde{q}_n} & RF_{n-1} \\ \downarrow \text{---} & & \downarrow \pi & \xleftarrow{t_n} & \downarrow \cong \\ \mathcal{K}'_n & \hookrightarrow & \mathcal{K}_n & \xrightarrow{q_n} & RF_{n-1} \end{array}$$

**Step 3** In order to show that the induced projection  $\pi : \tilde{\mathcal{H}}'_n \rightarrow \mathcal{H}'_n$  is an isomorphism, we need to investigate the structure of  $\tilde{\mathcal{H}}'_n$ . By Lemma 3.2, it is generated by the  $\chi_{in}^w$  for  $w \in \langle \chi_{nj} \rangle \cong \text{RF}_{n-1}$ , and the relations (R2) say exactly that these commute with each other. Thus  $\tilde{\mathcal{H}}'_n$  is abelian. Let us fix  $i$  and denote by  $\tilde{N}_i$  the subgroup generated by the  $\chi_{in}^w$ . It is the normal closure of  $\chi_{in}$  in the subgroup  $\tilde{M}_i$  generated by  $\chi_{in}$  and the  $\chi_{nj}$ . Relations (R1) and (R2) imply that  $\chi_{in}$  and the  $\chi_{nj}$  commute with their conjugates in  $M_i$ , which is thus a quotient of  $\text{RF}_n$ . In particular,  $\tilde{M}_i$  is nilpotent, and we can apply Proposition 5.4 to get that  $\tilde{N}_i$  is generated by Lyndon monomials in  $\chi_{in}$  and the  $\chi_{nj}$  containing  $\chi_{in}$ . We can even limit ourselves to the subset  $\text{Lynd}(\chi_{in}; (\chi_{nj})_j)$  of monomials without repetitions, the other ones being trivial by the argument above. Furthermore, the relations (R3) say exactly that among these, the ones containing  $\chi_{ni}$  vanish. Thus, the abelian group  $\tilde{N}_i$  is generated by  $\text{Lynd}(\chi_{in}; \chi_{n1}, \dots, \hat{\chi}_{ni}, \dots, \chi_{n,n-1})$ . Because of Lemma 5.6, we know that these monomials are sent to linearly independent elements in  $N_i$  (in fact, to a basis of this abelian group), so they must be a basis of  $\tilde{N}_i$ , and the projection  $\pi$  induced a isomorphism between  $\tilde{N}_i$  and  $N_i$ . The projection  $\pi : \tilde{\mathcal{H}}'_n \rightarrow \mathcal{H}'_n$ , being the direct product of these isomorphisms, is thus an isomorphism, which is the desired conclusion.  $\square$

**Remark 5.9** The same remarks made at the end of Section 1.2 for  $\text{RF}_n$  hold true for  $hP\Sigma_n$ : it is finitely generated and nilpotent (of class  $n - 1$ ), so it has a finite presentation. However, in order to write down such a finite presentation, we need a presentation of the free  $(n-1)$ -nilpotent group on  $n^2$  generators  $\chi_{ij}$ . We can then add to such a presentation the relations similar to (R1), (R2) and (R3) that are iterated brackets of the generators (of any shape) of length at most  $n - 1$  to get an explicit finite presentation of  $hP\Sigma_n$ . In other words, the latter relations give a finite presentation of  $hP\Sigma_n$  as an  $(n-1)$ -nilpotent group.

### 5.3 A presentation of the associated Lie ring

Using the above methods, one can also find a presentation of the Lie ring associated to  $hP\Sigma_n$ , similar to the presentation of  $\mathcal{L}(hP_n)$  given in Corollary 3.12.

**Proposition 5.10** *The Lie ring of  $hP\Sigma_n$  is generated by  $x_{ij}$  ( $1 \leq i \neq j \leq n$ ), under the relations*

$$\begin{aligned} [x_{ik} + x_{jk}, x_{ij}] &= 0 \quad \text{for } i, j, k \text{ pairwise distinct,} \\ [x_{ik}, x_{jk}] &= 0 \quad \text{for } i, j, k \text{ pairwise distinct,} \\ [x_{ij}, x_{kl}] &= 0 \quad \text{if } \{i, j\} \cap \{k, l\} = \emptyset, \end{aligned}$$

to which are added, for each  $m$ , the families of relations

$$[x_{im}, [x_{mi}, t]] = 0, \quad [x_{im}, [x_{jm}, t]] = 0, \quad [x_{im}, [x_{mi}, t]] = 0,$$

where, in each case,  $t$  describes Lie monomials in the  $x_{mk}$  ( $k < m$ ).

**Proof** Since it is very similar to the proof of Theorem 5.8, we only outline the proof. Let  $hp_n$  be the Lie ring defined by the presentation of the theorem. The relations are true for the classes of the  $\chi_{ij}$  in  $\mathcal{L}(hP\Sigma_n)$  (as direct consequences of the relations in the group  $hP\Sigma_n$ ), so  $x_{ij} \mapsto \bar{\chi}_{ij}$  defines a projection

$\pi$  from  $h\mathfrak{p}_n$  onto  $\mathcal{L}(hP\Sigma_n)$ . One shows that  $h\mathfrak{p}_n$  admits a decomposition similar to the decomposition of  $\mathcal{L}(hP\Sigma_n)$  described in [Theorem 3.8](#). Indeed, the morphism from  $h\mathfrak{p}_n$  to  $h\mathfrak{p}_{n-1}$  sending  $x_{ij}$  on  $x_{ij}$  if  $n \notin \{i, j\}$  and to 0 else is a well-defined projection  $p$ , which is split. From the relations, reasoning as in the proof of [Lemma 3.3](#), one checks that the  $x_{in}$  together with the  $x_{ni}$  generate an ideal of  $h\mathfrak{p}_n$ , which has to be the kernel  $\mathfrak{k}_n$  of  $p$ . They one argues exactly as in the proof of [Theorem 5.8](#) to show (using the first family of relations) that  $\mathfrak{k}_n$  decomposes as a semidirect product  $\mathfrak{k}'_n \rtimes R\mathcal{L}_{n-1}$ . Moreover, the projection  $\pi$  is compatible with the decompositions of  $h\mathfrak{p}_n$  and  $\mathcal{L}(hP\Sigma_n)$ . Using the five lemma, we see that we only have to check that  $\pi$  induces an isomorphism between  $\mathfrak{k}'_n$  and  $\prod \langle y_i \rangle$ . Since we know a basis of the target, whose elements are Lie monomials on the  $\bar{\chi}_{in}$  and  $\bar{\chi}_{ni}$ , we are left with showing that the corresponding Lie monomials on the  $x_{in}$  and  $x_{ni}$  generate  $\mathfrak{k}'_n$ . Like in the proof of [Theorem 5.8](#), the last two families of relations ensure exactly that, so  $\pi$  is indeed an isomorphism.  $\square$

**Remark 5.11** In the presentation, one can consider only the relations where  $t$  is a linear monomial of length at most  $m$ .

**Remark 5.12** It is a difficult open question, very much related to the Andreadakis problem for  $P\Sigma_n$ , to decide whether the first three relations (the linearized McCool relations) define a presentation of the Lie ring of  $P\Sigma_n$ . It is only known to hold rationally [[Berceanu and Papadima 2009](#)].

## Appendix Lyndon words and the free Lie algebra

For the comfort of the reader, we gather here some basic facts about Lyndon words. These describe a basis of the free Lie algebra, and we give a self-contained proof of this classical result involving as little machinery as possible. Our main sources for this appendix were Serre's lecture notes [[1965](#)] and Reutenauer's book [[2003](#), 5.1].

### A.1 Lyndon words

Let  $\mathcal{A}$  be a set (called an *alphabet*) endowed with a fixed total order. We denote by  $\mathcal{A}^*$  the free monoid generated by  $\mathcal{A}$ . Elements of  $\mathcal{A}^*$  are *words* in  $\mathcal{A}$ , that is, finite sequence of elements of  $\mathcal{A}$ . The set  $\mathcal{A}^*$  is endowed with the usual dictionary order induced by the order on  $\mathcal{A}$ .

The length of a word  $w$  is denoted by  $|w|$ . If  $v$  and  $w$  are words,  $v$  is a *suffix* (resp. a *prefix*) of  $w$  if there exists a word  $u$  such that  $w = uv$  (resp.  $w = vu$ ). It is called *proper* when it is nonempty and different from  $w$ .

**Definition A.1** The *standard factorization* of a word  $w$  of length at least 2 is the factorization  $w = uv$ , where  $v$  is the smallest proper suffix of  $w$ .

**Definition A.2** A *Lyndon word* is a nonempty word that is minimal among its nonempty suffixes.

**Lemma A.3** *If  $w = uv$  is a standard factorization, then  $v$  is a Lyndon word, and if  $w$  is Lyndon then so is  $u$ .*

**Proof** The fact that  $v$  is a Lyndon word is clear. Suppose that  $w$  is a Lyndon word. Let  $x$  be any proper suffix of  $u$ . Since  $uv = w < xv$ , if  $x$  is not a prefix of  $u$ , then  $u < x$ . Otherwise,  $u = xy$  for some nonempty  $y$ , but then  $xyv < xv$  implies  $yv < v$ , which contradicts the definition of  $v$ .  $\square$

The following proposition is the most basic result in the theory of Lyndon words:

**Proposition A.4** *Every word  $w \in \mathcal{A}^*$  factorizes uniquely as a product  $l_1 \cdots l_n$  where  $n$  is an integer, the  $l_i$  are Lyndon words and  $l_1 \geq l_2 \geq \cdots \geq l_n$ . We call this the **Lyndon factorization** of  $w$ .*

**Proof** We first prove unicity, by proving that in a factorization  $w = l_1 \cdots l_n$  into a nonincreasing product of Lyndon words,  $l_n$  is the smallest nonempty suffix of  $w$ . Indeed, let  $v$  be a suffix of  $w$ . Decompose  $v$  as  $yl_{k+1} \cdots l_n$ , where  $y$  is a nonempty suffix of  $l_k$  (possibly equal to  $l_k$ ). Then  $v \geq y \geq l_k \geq l_n$ .

We show existence by induction on the length of  $w$ . Take  $l_n$  to be the smallest nonempty suffix of  $w$ . Then  $w = w'l_n$ , and  $l_n$  is a Lyndon word. Moreover, a nonempty suffix of  $w'$  cannot be strictly smaller than  $l_n$ . Indeed, if  $y$  is a nonempty suffix of  $w'$  such that  $y < l_n$ , then either  $y$  is a (proper) prefix of  $l_n$  or  $yl_n < l_n$ . The second case contradicts the definition of  $l_n$ . In the first case, by definition of  $l_n$ , we get  $yl_n > l_n = yu$ , whence  $l_n > u$ . Thus both cases contradict the definition of  $l_n$ ; we must have  $y \geq l_n$ . As a consequence, a factorization of  $w'$  satisfying the conditions of the proposition gives such a factorization for  $w$ , whence the conclusion.  $\square$

Proposition A.4 allows us to identify the abelian group  $\mathbb{Z}\mathcal{A}^*$  with the symmetric algebra  $S_{\mathbb{Z}}^*(\text{Lynd})$ . Note that this linear identification does not preserve the ring structure, since the Lyndon factorization of a product  $uv$  need not be the product of the Lyndon factorization of  $u$  with that of  $v$ .

## A.2 The Lyndon basis of the free Lie algebra

In the sequel,  $V = \mathbb{Z}\{\mathcal{A}\}$  is the free abelian group generated by the alphabet  $\mathcal{A}$ . We denote by  $\mathfrak{L}V$  the free Lie algebra on  $V$  and by  $TV$  the free associative algebra on  $V$ . Recall that their universal properties imply that  $TV$  is the enveloping algebra of  $\mathfrak{L}V$ . We denote by  $\iota: \mathfrak{L}V \rightarrow TV$  the canonical Lie morphism between them. Note that we do not know a priori that this map is injective (we do not assume the PBW theorem to be known).

Define an application  $w \mapsto P_w$  from the set Lynd of Lyndon word on  $\mathcal{A}$  to  $\mathfrak{L}V$  as follows:

- Take  $P_a := a \in V$  for any letter  $a \in \mathcal{A}$ .
- If  $w$  is a Lyndon word, consider its standard factorization  $w = uv$  and define  $P_w$  to be  $[P_u, P_v] \in \mathfrak{L}V$ .

**Lemma A.5** (standard factorization of a product of Lyndon words) *Let  $u$  and  $v$  be Lyndon words. Then  $uv$  is a Lyndon word if and only if  $u < v$ . Moreover, suppose that  $u < v$ , and denote by  $u = xy$  the standard factorization of  $u$ , if  $u$  is not a letter. Then the standard factorization of  $uv$  is  $u \cdot v$  if and only if  $u$  is a letter or  $v \leq y$ .*

**Proof** If  $uv$  is a Lyndon word, then  $u < uv < v$ . Conversely, suppose that  $u < v$ . Then either  $uv < v$  or  $u$  is a prefix of  $v$ . But in this second case,  $v = uw$ , and  $v < w$  implies that  $uv < uw = v$ , so in both cases  $uv < v$ . Now, take a proper suffix  $w$  of  $uv$ . If  $w$  is a suffix of  $v$ , then  $w \geq v > uv$ . If not, then  $w = w'v$  with  $w'$  a proper suffix of  $u$ . Then  $u < w'$  implies  $uv < w'v = w$ , finishing the proof that  $uv$  is a Lyndon word.

If  $u$  is a letter, then  $v$  is clearly the smallest proper suffix of  $uv$ . Let us assume that  $u$  is not a letter. Suppose that  $v \leq y$ . A proper suffix of  $uv$  is either a suffix of  $v$ , which is greater than  $v$ , or of the form  $wv$ , where  $w$  is a proper suffix of  $u$ . In the latter case, since  $y$  is the smallest proper suffix of  $u$ , we have  $v \leq y \leq w < wv$ . This shows that  $v$  is the smallest proper suffix of  $uv$  in this case. Conversely, if  $v > y$ , then  $yv$  is a Lyndon word by the first part of the proof. Hence  $yv < v$ , so  $v$  is not the smallest proper suffix of  $uv$  in this case. □

The following proposition and its proof are adapted from [Serre 1965, Theorem 5.3]. The proof is arguably the most technical one in the present appendix:

**Proposition A.6** *The  $P_w$  for  $w \in \text{Lynd}$  linearly generate  $\mathfrak{L}V$ .*

**Proof** We only need to show that the  $\mathbb{Z}$ -module generated by the  $P_w$  is a Lie subalgebra. We show that if  $u$  and  $v$  are Lyndon words, then  $[P_u, P_v]$  is a linear combination of  $P_w$ , with  $|w| = |u| + |v|$  and  $w < \max(u, v)$ , by induction on  $|u| + |v|$  and on  $\max(u, v)$ . To begin with, if  $u$  and  $v$  are letters, then we can suppose that  $u < v$  (otherwise, use the antisymmetry relation). Then  $[P_u, P_v] = P_{uv}$ , and  $uv < v$ .

Now, take  $(u, v)$  such that  $|u| + |v| > 2$ , and suppose that our claim is proven for every  $(u', v')$  such that  $|u'| + |v'| < |u| + |v|$ , or  $|u'| + |v'| = |u| + |v|$  and  $\max(u', v') < \max(u, v)$ . Using antisymmetry if needed, we can assume that  $u < v$ . We then use Lemma A.5. When  $u$  is not a letter, consider the standard factorization  $u = xy$  of  $u$ . If  $u$  is a letter or  $y \geq v$ , then  $u \cdot v$  is the standard factorization of  $uv$ , whence  $[P_u, P_v] = P_{uv}$ , and  $uv < v$ , proving our claim. Suppose that  $y < v$ . Then

$$[P_u, P_v] = [[P_x, P_y], P_v] = [[P_x, P_v], P_y] + [P_x, [P_y, P_v]].$$

Since  $|x|, |y| < |u|$ , we can use the induction hypothesis to write  $[P_x, P_v]$  (resp.  $[P_y, P_v]$ ) as a linear combination of  $P_w$  (resp.  $P_t$ ) such that  $|w| = |x| + |v|$  (resp.  $|t| = |y| + |v|$ ), and  $w < v$  (resp.  $t < v$ ). Then, using that  $x, y < v$  (since  $x < xy = u < y < v$ ), we can apply the induction hypothesis to  $[P_w, P_y]$  (resp. to  $[P_x, P_t]$ ) to prove our claim, ending the proof of the proposition. □

The application  $w \mapsto P_w$  extends to a map from  $\mathcal{A}^*$  to  $TV$  defined as follows:

- Take  $P_a := a \in V$  for any letter  $a \in \mathcal{A}$ .
- If  $w$  is a Lyndon word, consider its standard factorization  $w = uv$  and define  $P_w$  to be  $[P_u, P_v] \in \mathcal{L}V$ .
- If  $w$  is any word, consider its Lyndon factorization  $w = l_1 \cdots l_n$ . Define  $P_w$  to be  $P_{l_1} \cdots P_{l_n} \in TV$ .

The next lemma [Reutenauer 2003, Theorem 5.1], which says that the expression of the  $P_w$  in terms of associative monomials is governed by a triangular matrix, will play a key role in what follows.

**Lemma A.7** *For any word  $w$ , the polynomial  $P_w$  is the sum of  $w$  and a linear combination of (strictly) greater words having the same length as  $w$ .*

**Proof** Note that if  $l$  is a Lyndon word and  $l = uv$  with  $u$  and  $v$  nonempty, then  $uv = l < v < vu$ .

We use this to show the lemma for Lyndon words, by induction on their length. For letters, the result is obvious. Let  $l$  be a Lyndon word, and consider its standard factorization  $l = uv$ . Then  $u$  and  $v$  are Lyndon words, and  $u < v$  (Lemmas A.3 and A.5). If the result is true for  $u$  and  $v$ , then  $P_l = [P_u, P_v]$  is a linear combination of elements of the form  $[s, t] = st - ts$ , where  $|s| = |u|$ ,  $|t| = |v|$ ,  $s \geq u$  and  $t \geq v$ . Then  $ts \geq vu > uv$ , and  $st \geq uv$ , with equality if and only if  $s = u$  and  $t = v$ . Thus the word  $l = uv$  appears with coefficient 1 in the decomposition of  $P_l$ , and  $P_l - l$  is a linear combination of greater words, of the same length as  $l$ , which proves our claim.

Now, if  $w$  is any word, consider its Lyndon factorization  $w = l_1 \cdots l_n$ . Then  $P_w := P_{l_1} \cdots P_{l_n}$  is a linear combination of  $x_1 \cdots x_n$ , where each  $x_i$  is a word satisfying  $|x_i| = |l_i|$  and  $x_i \geq l_i$ . As a consequence,  $|x_1 \cdots x_n| = |l_1 \cdots l_n|$ , and  $x_1 \cdots x_n \geq l_1 \cdots l_n$ , with equality if and only if each  $x_i$  is equal to  $l_i$ . This last case only appears with coefficient 1, so the lemma is proved. □

The above application extends to a linear map  $P : \mathbb{Z}\mathcal{A}^* \rightarrow TV$ .

**Proposition A.8** *The application  $P : \mathbb{Z}\mathcal{A}^* \rightarrow TV$  defined above is injective.*

**Proof** Let  $m$  be a linear combination of words in the kernel of  $P$ . Suppose that  $w$  is such that no word smaller than  $w$  appears in  $m$ . Let  $\lambda$  be the coefficient of  $w$  in  $m$ . Then by Lemma A.7,  $\lambda$  is also the coefficient of  $w$  in  $P_m = 0$ , so it must be trivial. Thus, by induction, all coefficients of  $m$  have to be trivial, whence  $m = 0$  and  $P$  is injective. □

We can now sum this up as the main result of this appendix:

**Theorem A.9** *The map  $P$  induces a graded linear isomorphism*

$$\mathbb{Z}\{\text{Lynd}\} \cong \mathcal{L}V.$$

*Otherwise said, the family  $(P_w)_{w \in \text{Lynd}}$  is a linear basis of  $\mathcal{L}V$ .*

**Proof** The  $P_w$  generate  $\mathcal{L}V$  (Proposition A.6) and, since their images in  $TV$  are linearly independent (Proposition A.8), they must be linearly independent. □



### A.3 Primitive elements and the Milnor–Moore theorem

In proving the previous result, we have only used basic linear algebra, and the combinatorics of Lyndon words. In order to convince the reader of how powerful these techniques are, we will now recover the Milnor–Moore theorem for the algebra  $TV$ , using not much more machinery. The only additional tools we need are coalgebra structures and primitive elements.

The free commutative ring on the free abelian group  $V$  is denoted by  $S^*(V)$ . It is endowed with its usual Hopf algebra structure, whose coproduct is the only algebra morphism  $\Delta: S^*(V) \rightarrow S^*(V) \otimes S^*(V)$  sending each element  $v$  of  $V$  to  $v \otimes 1 + 1 \otimes v$ . That is, it is the only bialgebra structure on  $S^*(V)$  such that  $V$  consists of primitive elements. In fact, these are the only primitive elements in  $S^*(V)$  [Serre 1965, Theorem 5.4]:

**Proposition A.10** *The set of primitive elements of  $S^*(V)$  is  $V$ .*

**Proof** By definition of the coproduct of  $S^*(V)$ , the subspace  $V$  is made of primitive elements. To show the converse, it is helpful to see  $S^*(V)$  as the algebra  $\mathbb{Z}[X_i]$  of polynomials in indeterminates  $X_i$ . Then  $S^*(V) \otimes S^*(V)$  identifies with  $\mathbb{Z}[X'_i, X''_i]$ , and the coproduct sends  $X_i$  to  $X'_i + X''_i$ . Since it is an algebra morphism, it sends a polynomial  $f(X_i)$  to  $f(X'_i + X''_i)$ . Thus primitive elements are those  $f$  such that  $f(X'_i + X''_i) = f(X'_i) + f(X''_i)$ , ie additive ones. But since we work over  $\mathbb{Z}$ , these are only the linear ones, which is the desired conclusion.  $\square$

The algebra  $TV$  is endowed with a Hopf structure defined exactly as the one for  $S^*V$ : it is the unique bialgebra structure such that elements of  $V$  are primitive ones. Since primitive elements are a Lie subalgebra, they contain the Lie subalgebra generated by  $V$  (which is the image  $\iota(\mathfrak{L}V)$  of the canonical morphism  $\iota: \mathfrak{L}V \rightarrow TV$ ).

Recall that [Proposition A.4](#) allows us to identify  $\mathbb{Z}\mathcal{A}^*$  with the symmetric algebra  $S^*_{\mathbb{Z}}(\text{Lynd})$ . We will show the following:

**Theorem A.11** (Milnor–Moore) *The application  $P: S^*_{\mathbb{Z}}(\text{Lynd}) \rightarrow TV$  defined in [Section A.2](#) is an isomorphism of coalgebras.*

**Proof** Injectivity has already been shown ([Proposition A.8](#)). Let us first prove surjectivity. Let  $p \neq 0$  be a homogeneous element of  $TV$ . Let  $w$  be the smallest monomial appearing in  $p$ , with coefficient  $\lambda$ . Then  $p - \lambda P_w$  is homogeneous and contains only monomials greater than  $w$  (see [Lemma A.7](#)). By repeating this process, we can write  $p$  as a linear combination of  $P_w$ . Indeed, this process stops, since we consider only the finite set of words of fixed length (equal to the degree of  $p$ ) whose letters appear in some monomial of  $p$ . This proves that  $P$  is surjective.



We are left to show that the application  $P : w \mapsto P_w$  preserves the coproduct. We first remark that if  $l$  is a Lyndon word, then  $l$  is primitive in  $S_{\mathbb{Z}}^*(\text{Lynd})$ , and  $P_l \in \iota(\mathcal{L}V)$  is primitive in  $TV$ . For any word  $w$ , consider its Lyndon factorization  $w = l_1 \cdots l_n$ . Then we can write

$$\begin{aligned} \Delta(P_w) &= \Delta(P_{l_1}) \cdots \Delta(P_{l_n}) = (P_{l_1} \otimes 1 + 1 \otimes P_{l_1}) \cdots (P_{l_n} \otimes 1 + 1 \otimes P_{l_n}) \\ &= \sum_{\underline{n} = X \sqcup Y} P_{l_{x_1}} \cdots P_{l_{x_p}} \otimes P_{l_{y_1}} \cdots P_{l_{y_q}}, \end{aligned}$$

where the sum is over all partitions of the set  $\underline{n} = \{1, \dots, n\}$  into two subsets  $X = \{x_1 < \cdots < x_p\}$  and  $Y = \{y_1 < \cdots < y_q\}$ . As a consequence,

$$\begin{aligned} \Delta(P_w) &= \sum_{\underline{n} = X \sqcup Y} P_{l_{x_1} \cdots l_{x_p}} \otimes P_{l_{y_1} \cdots l_{y_q}} \\ &= (P \otimes P) \left( \sum_{\underline{n} = X \sqcup Y} l_{x_1} \cdots l_{x_p} \otimes l_{y_1} \cdots l_{y_q} \right) \\ &= (P \otimes P)(\Delta(l_1) \cdots \Delta(l_n)) = (P \otimes P)(\Delta(w)). \quad \square \end{aligned}$$

**Corollary A.12** *The canonical map  $\iota : \mathcal{L}V \rightarrow TV$  identify  $\mathcal{L}V$  with the Lie algebra of primitive elements in  $TV$ .*

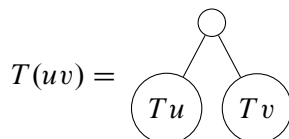
**Proof** Thanks to Theorems A.9 and A.11, this map identifies with  $\mathbb{Z}\{\text{Lynd}\} \rightarrow S_{\mathbb{Z}}^*(\text{Lynd})$ . But Proposition A.10 ensures that the set of primitive elements of the coalgebra  $S_{\mathbb{Z}}^*(\text{Lynd})$  is exactly  $\mathbb{Z}\{\text{Lynd}\}$ , whence the result.  $\square$

**Remark A.13** Neither our identification of the free abelian group  $\mathbb{Z}\{\text{Lynd}\}$  with the primitives of  $TV$  nor our proof of Theorem A.11 requires the use of the fact that Lyndon words generate  $\mathcal{L}V$  (Proposition A.6); we only used that they are linearly independent (Proposition A.8) for that. The full strength of Theorem A.9 is only used to see that  $P : \mathbb{Z}\mathcal{A}^* \hookrightarrow TV$  coincides with  $\iota : \mathcal{L}V \rightarrow TV$  (whence Corollary A.12).

### A.4 Linear trees

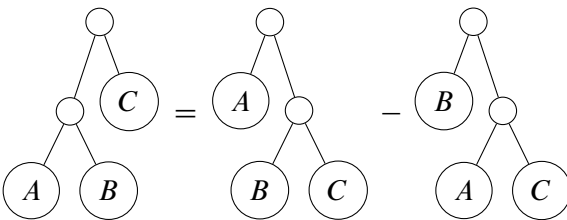
The free Lie algebra can be seen as a quotient of the free abelian group  $\mathbb{Z}\mathcal{M}(\mathcal{A})$  on the free magma  $\mathcal{M}(\mathcal{A})$  on  $\mathcal{A}$  by antisymmetry and the Jacobi identity. Elements of the free magma can be seen as parenthesized words in  $\mathcal{A}$ , or as finite rooted planar binary trees, whose leaves are indexed by elements of  $\mathcal{A}$ . The images of elements of the free magma in  $\mathcal{L}V$  are called *Lie monomials*.

Lyndon words encode a family of rooted binary trees whose leaves are indexed by letters. Precisely, if  $w$  is a Lyndon word, the tree  $T(w)$  is just one leaf indexed by  $w$ , if  $w$  is a letter. If not, take the standard factorization  $w = uv$ . Then  $T(w)$  is given by a root, a left son  $T(u)$  and a right son  $T(v)$ :



The Lyndon basis of the free Lie algebras are the Lie monomials  $P_w$  obtained from such trees by interpreting nodes as Lie brackets. We call these *Lyndon monomials*

One can consider another family of Lie monomials, called *linear Lie monomials*, given by linear trees, that is, monomials which are letters or of the form  $[y_1, \dots, y_n]$  ( $= [y_1, [y_2, [\dots [y_{n-1}, y_n] \dots]]$ ). It is easy to see, by induction, using the Jacobi identity, that these generate  $\mathfrak{L}V$ . In fact, the Jacobi identity can be written as

(A-1) 

Using this as a rewriting rule (from left to right), one can write any tree (that is, any Lie monomial) as a linear combination of trees whose left son is a leaf. Applying the induction hypothesis to the right sons, one gets a linear combination of linear trees.

There are  $n!$  linear Lie monomials in degree  $n$ , which is clearly strictly greater than the number of Lyndon words of length  $n$ , so they must be linearly dependent. It is the need to control this redundancy that leads us to consider Lyndon words (or, more generally, Hall sets).

**Lemma A.14** *Any Lie monomial is a linear combination of linear Lie monomials with the same letters (counted with repetitions). Also, it is a linear combination of Lyndon monomials with the same letters.*

**Proof** The first part follows from the rewriting process that we have just described. The second one is a bit trickier: although we know that a decomposition into a linear combination of Lyndon monomials *exists* (Proposition A.6), we did not give an algorithm to compute it. However, we can use a homogeneity argument as follows:  $\mathbb{Z}\mathcal{M}(\mathcal{A})$  is  $\mathbb{N}\{\mathcal{A}\}$ -graded, the degree of an element of the free magma  $\mathcal{M}(\mathcal{A})$  being its image in the free commutative monoid  $\mathbb{N}\{\mathcal{A}\}$  (which counts the number of appearance of each letter in a given nonassociative word). Moreover, the antisymmetry and the Jacobi relations are homogeneous with respect to this degree, so that the quotient  $\mathfrak{L}[\mathcal{A}]$  is again a graded abelian group with respect to this degree. As a consequence, if we write a Lie monomial  $m$  of degree  $d$  as a linear combination of Lyndon monomials, taking the homogeneous component of degree  $d$  results in an expression of  $m$  as a linear combination of Lyndon monomials of degree  $d \in \mathbb{N}\{\mathcal{A}\}$ , as claimed. □

We remark that the expression of  $m$  obtained in the proof by taking the homogeneous component must in fact must be the same as the first one, because of Theorem A.9.

Linear trees can be used to define a basis of the reduced free Lie ring  $R\mathfrak{L}[n]$  which could be used to replace the Lyndon basis in all our work (this is in fact the point of view used in [Meilhan and Yasuhara 2019]):

**Lemma A.15** For all integer  $k \geq 2$ , a basis of  $R\mathcal{L}[n]_k$  is given by Lie monomials which are letters or of the form  $[y_{i_1}, \dots, y_{i_k}]$  where the  $i_j \leq n$  are pairwise distinct and satisfy  $i_k = \max_j(i_j)$ .

**Proof** Using antisymmetry, one sees that up to a sign, any Lie monomial without repetition is equal to a Lie monomial with the same letter where the right-most factor (the right-most leaf of the corresponding tree) bears the maximal index. Then we can use the rewriting rule (A-1) to get a linear combination of linear trees, and the right-most leaf stays the same throughout the process, as does the set of letters used. This shows that Lie monomials of the form described in the lemma generate the abelian group  $R\mathcal{L}[n]_k$ . Moreover, there are  $(k-1)! \binom{n}{k}$  such monomials, which is already known to be the rank of  $R\mathcal{L}[n]_k$  (Proposition 1.9); hence this family must be a basis of  $R\mathcal{L}[n]_k$ .  $\square$

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# ALGEBRAIC & GEOMETRIC TOPOLOGY

Volume 24 Issue 3 (pages 1225–1808) 2024

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Models of $\mathcal{G}$ -spectra as presheaves of spectra	1225
BERTRAND J GUILLOU and J PETER MAY	
Milnor invariants of braids and welded braids up to homotopy	1277
JACQUES DARNÉ	
Morse–Bott cohomology from homological perturbation theory	1321
ZHENGYI ZHOU	
The localization spectral sequence in the motivic setting	1431
CLÉMENT DUPONT and DANIEL JUTEAU	
Complex hypersurfaces in direct products of Riemann surfaces	1467
CLAUDIO LLOSA ISENRICH	
The $K(\pi, 1)$ conjecture and acylindrical hyperbolicity for relatively extra-large Artin groups	1487
KATHERINE M GOLDMAN	
The localization of orthogonal calculus with respect to homology	1505
NIALL TAGGART	
Bounded subgroups of relatively finitely presented groups	1551
EDUARD SCHESLER	
A topological construction of families of Galois covers of the line	1569
ALESSANDRO GHIGI and CAROLINA TAMBORINI	
Braided Thompson groups with and without quasimorphisms	1601
FRANCESCO FOURNIER-FACIO, YASH LODHA and MATTHEW C B ZAREMSKY	
Oriented and unitary equivariant bordism of surfaces	1623
ANDRÉS ÁNGEL, ERIC SAMPERTON, CARLOS SEGOVIA and BERNARDO URIBE	
A spectral sequence for spaces of maps between operads	1655
FLORIAN GÖPPL and MICHAEL WEISS	
Classical homological stability from the point of view of cells	1691
OSCAR RANDAL-WILLIAMS	
Manifolds with small topological complexity	1713
PETAR PAVEŠIĆ	
Steenrod problem and some graded Stanley–Reisner rings	1725
MASAHIRO TAKEDA	
Dehn twists and the Nielsen realization problem for spin 4–manifolds	1739
HOKUTO KONNO	
Sequential parametrized topological complexity and related invariants	1755
MICHAEL FARBER and JOHN OPREA	
The multiplicative structures on motivic homotopy groups	1781
DANIEL DUGGER, BJØRN IAN DUNDAS, DANIEL C ISAKSEN and PAUL ARNE ØSTVÆR	
Coxeter systems with 2–dimensional Davis complexes, growth rates and Perron numbers	1787
NAOMI BREDON and TOMOSHIGE YUKITA	