THE JOHNSON–MORITA THEORY FOR THE HANDLEBODY GROUP

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Abstract. The Johnson–Morita theory is an algebraic approach to the mapping class group of a surface Σ, in which one considers its action on the successive nilpotent quotients of the fundamental group $\pi = \pi_1(\Sigma)$. In this paper, we develop an analogue of this theory for the handlebody group, i.e. the mapping class group of a handlebody V bounded by a surface Σ, by considering its action on the pair (π, A), where A denotes the kernel of the homomorphism induced by the inclusion of Σ in V. We give a detailed study of the analogues of the Johnson filtration and the Johnson homomorphisms that arise in this new context. In particular, we obtain new representations of subgroups of the handlebody group into spaces of oriented trees with beads.

Contents

1. Introduction

The *Johnson–Morita theory* studies the mapping class group of a surface by studying its action on the lower central series of the fundamental group of the surface. In this paper, we introduce an analogue of this theory for the handlebody group.

1.1. **The Johnson–Morita theory for the mapping class group.** We first briefly outline the original Johnson–Morita theory. Let Σ be a compact, connected, oriented surface with one boundary component. Let $\mathcal{M} := \mathcal{M}(\Sigma, \partial\Sigma)$ be the mapping class group of Σ relative to $\partial\Sigma$.

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By a classical result of Dehn and Nielsen, the canonical action of $\mathcal{M}$ on $\pi := \pi_1(\Sigma, \star)$, with base point $\star \in \partial\Sigma$, is faithful. Thus, $\mathcal{M}$ embeds into $\mathrm{Aut}(\pi)$. Let

$$\pi = \Gamma_1\pi \geq \Gamma_2\pi \geq \cdots \geq \Gamma_k\pi \geq \cdots$$

be the lower central series of π. Its associated graded Lie algebra is isomorphic to the free Lie algebra $\mathrm{Lie}(H)$ on $H := H_1(\Sigma; \mathbb{Z})$.

The *Johnson filtration* of $\mathcal{M}$ is the decreasing sequence of subgroups

$$\mathcal{M} = \mathcal{M}_0 \geq \mathcal{M}_1 \geq \cdots \geq \mathcal{M}_k \geq \cdots$$

defined by

$$\begin{aligned} \mathcal{M}_k \quad &:= \quad \ker\big(\mathcal{M} \longrightarrow \mathrm{Aut}(\pi/\Gamma_{k+1}\pi)\big) && (1.1)\\ &= \quad \big\{ f \in \mathcal{M} \mid f(x)x^{-1} \in \Gamma_{k+i}\pi \text{ for all } x \in \Gamma_i\pi, i \geq 1 \big\}. && (1.2)\end{aligned}$$

Johnson studied its first few terms (see [Jo83]). The first term $\mathcal{I} := \mathcal{M}_1$, known as the *Torelli group*, is the subgroup of $\mathcal{M}$ acting trivially on H. Morita [Mo93] studied the Johnson filtration systematically. It has trivial intersection

$$\bigcap_{k \geq 1} \mathcal{M}_k = \{1\}, \tag{1.3}$$

and it is an *N-series*, i.e., we have

$$\big[\mathcal{M}_k, \mathcal{M}_l\big] \subset \mathcal{M}_{k+l} \quad \text{for all } k, l \geq 1. \tag{1.4}$$

An important problem is to compute the associated graded Lie algebra

$$\overline{\mathcal{M}}_+ := \bigoplus_{k \geq 1} \mathcal{M}_k/\mathcal{M}_{k+1}.$$

The conjugation of $\mathcal{M}$ on $\mathcal{I}$ induces an action of the symplectic group $\mathrm{Sp}(H) \simeq \mathcal{M}/\mathcal{I}$ on $\overline{\mathcal{M}}_+$. Here the symplectic form $\omega : H \times H \to \mathbb{Z}$ is the homology intersection form of Σ.

By works of Johnson, Morita and others, the structure of $\overline{\mathcal{M}}_k = \mathcal{M}_k/\mathcal{M}_{k+1}$ is well understood for $k = 1, 2$, and so is its rationalization $\overline{\mathcal{M}}_k \otimes \mathbb{Q}$ for some higher values of k in relation with Hain's computation [Ha97] of the Malcev Lie algebra of $\mathcal{I}$ (see [Mo99]). The general procedure to determine the abelian group $\overline{\mathcal{M}}_k$ for $k \geq 1$ is as follows. For any $f \in \mathcal{M}_k$ define a map $\tau_k(f) : \mathrm{Lie}(H) \to \mathrm{Lie}(H)$ by

$$\tau_k(f)([x]_i) = \big[f(x)x^{-1}\big]_{i+k} \quad (x \in \Gamma_i\pi, i \geq 1). \tag{1.5}$$

(Here, $[y]_j \in \Gamma_j\pi/\Gamma_{j+1}\pi = \mathrm{Lie}_j(H)$ denotes the class of $y \in \Gamma_j\pi$.) The map $\tau_k(f)$ vanishes if and only if $f \in \mathcal{M}_{k+1}$. Furthermore, $\tau_k(f)$ is a derivation of degree k and, since f fixes $\zeta := [\partial\Sigma] \in \pi$, the map $\tau_k(f)$ vanishes on $[\zeta]_2 \in \mathrm{Lie}_2(H) \simeq \Lambda^2 H$, which is dual to the intersection form ω on H. Thus, for every $k \geq 1$, we get an injective homomorphism

$$\overline{\tau}_k : \overline{\mathcal{M}}_k \longrightarrow \mathrm{Der}_k^\omega\big(\mathrm{Lie}(H)\big) := \big\{ d \in \mathrm{Der}_k\big(\mathrm{Lie}(H)\big) : d([\zeta]_2) = 0 \big\},$$

which is called the *k-th Johnson homomorphism*. All these homomorphisms τ_k, for $k \geq 1$, form an injective $\mathrm{Sp}(H)$-equivariant Lie algebra homomorphism

$$\overline{\tau}_+ := (\overline{\tau}_k)_{k\geq 1} : \overline{\mathcal{M}}_+ \longrightarrow \mathrm{Der}_+^\omega\big(\mathrm{Lie}(H)\big) := \bigoplus_{k\geq 1} \mathrm{Der}_k^\omega\big(\mathrm{Lie}(H)\big) \tag{1.6}$$

of $\overline{\mathcal{M}}_+$ into the Lie algebra of *symplectic derivations* of positive degree.

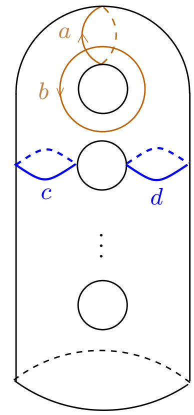
Example 1.1. Consider the first Johnson homomorphism

$$\tau_1 : \mathcal{M}_1 = \mathcal{I} \longrightarrow \mathrm{Der}_1^\omega\big(\mathrm{Lie}(H)\big) \simeq \Lambda^3 H.$$

The group $\mathcal{I}$ is generated by opposite Dehn twists $T_c T_d^{-1}$ along pairs of simple closed curves c and d cobounding a subsurface S of Σ [Jo79]. For such a pair (c,d), we have

$$\tau_1\big(T_c T_d^{-1}\big) = \pm\, \omega_S \wedge [c] \in \Lambda^3 H, \tag{1.7}$$

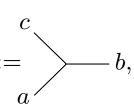
where $\omega_S \in \Lambda^2 H$ is dual to the intersection form of S (in the example on the right of genus 1, $\omega_S = a \wedge b$). This formula is crucial in the proof of the surjectivity of τ_1 [Jo80], which implies that $\overline{\mathcal{M}}_1 \simeq \Lambda^3 H$.

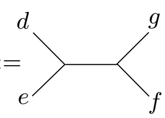


The computation of $\overline{\mathcal{M}}_2$ was carried out by Morita [Mo89]. Yet, in degree $k \geq 2$, it is much easier to work with rational coefficients. Since $\mathrm{Der}_+^\omega\big(\mathrm{Lie}(H)\big)$ is torsion-free, it embeds into $\mathrm{Der}_+^\omega\big(\mathrm{Lie}(H)\big) \otimes \mathbb{Q} = \mathrm{Der}_+^\omega\big(\mathrm{Lie}(H^\mathbb{Q})\big)$, the Lie $\mathbb{Q}$-algebra of positive-degree symplectic derivations of the free Lie $\mathbb{Q}$-algebra $\mathrm{Lie}(H^\mathbb{Q})$ on $H^\mathbb{Q} := H_1(\Sigma;\mathbb{Q})$. The latter has a diagrammatic description, which is implicit in [Ko93] and appears e.g. in [HP03] and [GL05]: there is an isomorphism of graded Lie $\mathbb{Q}$-algebras

$$\mathrm{Der}_+^\omega\big(\mathrm{Lie}(H^\mathbb{Q})\big) \simeq \mathcal{D}(H^\mathbb{Q}), \tag{1.8}$$

where $\mathcal{D}(H^\mathbb{Q})$ is the $\mathbb{Q}$-vector space generated by "oriented trivalent trees" with leaves colored by $H^\mathbb{Q}$. The Lie bracket of $\mathcal{D}(H^\mathbb{Q})$ is defined by gluing leaves to leaves using the pairing ω. For instance, the generators of $\mathcal{D}(H^\mathbb{Q})$ are

$\mathsf{Y}_{a,b,c} :=$ 

, $\mathsf{H}_{d,e,f,g} :=$ 

(with $a, b, \ldots, g \in H^\mathbb{Q}$)

in degrees 1 and 2, respectively, and the Lie bracket in degree $1+1$ is given by

$$\begin{aligned}
\big[\mathsf{Y}_{a,b,c}, \mathsf{Y}_{u,v,w}\big] \quad = \quad & \omega(a,u)\,\mathsf{H}_{b,c,v,w} + \omega(b,u)\,\mathsf{H}_{c,a,v,w} + \omega(c,u)\,\mathsf{H}_{a,b,v,w} \\
& + \omega(a,v)\,\mathsf{H}_{b,c,w,u} + \omega(b,v)\,\mathsf{H}_{c,a,w,u} + \omega(c,v)\,\mathsf{H}_{a,b,w,u} \\
& + \omega(a,w)\,\mathsf{H}_{b,c,u,v} + \omega(b,w)\,\mathsf{H}_{c,a,u,v} + \omega(c,w)\,\mathsf{H}_{a,b,u,v}.
\end{aligned} \tag{1.9}$$

This Lie bracket in $\mathcal{D}(H^\mathbb{Q})$ and formula (1.6) in degree 1 allow for explicit computations of τ_k in every degree $k > 1$ since, according to Hain [Ha97], the space $(\Gamma_k \mathcal{I}/\Gamma_{k+1}\mathcal{I}) \otimes \mathbb{Q}$ surjects onto $\overline{\mathcal{M}}_k \otimes \mathbb{Q}$.

To conclude this quick overview of the Johnson–Morita theory for the mapping class group, let us recall that all the Johnson homomorphisms τ_k for $k \geq 1$ unify into a single map

$$\varrho^\theta : \mathcal{I} \longrightarrow \widehat{\mathrm{Der}}_+^\omega\big(\mathrm{Lie}(H^\mathbb{Q})\big), \tag{1.10}$$

where the hat $\widehat{\ }$ denotes the degree-completion. The map ϱ^θ induces the rationalization of (1.6) at the graded level and we can regard ϱ^θ as an "infinitesimal" version of the canonical action of $\mathcal{I}$ on π. To define ϱ^θ we need a "symplectic expansion" θ of π, which manifests formality of the free group π. Indeed θ identifies the Malcev Lie algebra of π with the degree-completed free Lie algebra on $H^\mathbb{Q}$. Although ϱ^θ heavily depends on the choice of θ, it enjoys several properties. It is a group embedding if the target is endowed with the Baker–Campbell–Hausdorff

(BCH) product associated to the Lie bracket and, besides the property of determining all the Johnson homomorphisms, the map ϱ^θ gives (for an appropriate choice of θ) the tree-level of the representation of the Torelli group that is induced by the universal finite-type invariant of 3-manifolds [Mas12].

1.2. **Johnson–Morita theory for extended N-series.** In this paper, we develop an analogue of the Johnson–Morita theory for the *handlebody group*, i.e. the mapping class group of a 3-dimensional handlebody V.

The possibility of such a theory has been mentioned in [HM18, Ex. 10.9] as an instance of a general framework of extended N-series and extended graded Lie algebras, see Section 2. An *extended N-series* $K_* = (K_m)_{m\geq 0}$ is a descending filtration

$$K_0 \geq K_1 \geq \cdots \geq K_m \geq \cdots$$

of a group K_0 satisfying $[K_m, K_n] \subset K_{m+n}$ for all $m, n \geq 0$. An *action* of a group $\mathcal{G}$ on the extended N-series K_* is an action of $\mathcal{G}$ on K_0 such that $g(K_m) = K_m$ for all $g \in \mathcal{G}$ and $m \geq 0$. Similarly to (1.2), the *Johnson filtration*

$$\mathcal{G} = \mathcal{G}_0 \geq \mathcal{G}_1 \geq \mathcal{G}_2 \geq \cdots$$

is defined by

$$\mathcal{G}_m := \bigcap_{j\geq 0} \mathcal{G}_m^j, \quad \text{where } \mathcal{G}_m^j := \left\{ g \in \mathcal{G} : g(x)x^{-1} \in K_{m+j} \text{ for all } x \in K_j \right\}$$

but, in contrast with (1.1), we do not necessarily have $\mathcal{G}_m = \mathcal{G}_m^1$. As in the case of the mapping class group, this generalized Johnson filtration is an N-series and so has an associated graded $\overline{\mathcal{G}}_+$.

To the extended N-series $K_* = (K_m)_{m\geq 0}$ is associated the *extended graded Lie algebra* $\overline{K}_\bullet$, which is the pair of the graded Lie algebra $\overline{K}_+ = \bigoplus_{m\geq 1} K_m/K_{m+1}$ in positive degrees and the group $\overline{K}_0 = K_0/K_1$ in degree 0, the latter acting on the former by graded Lie algebra automorphisms. For $k \geq 1$, a *derivation* $d = (d_0, d_+)$ of $\overline{K}_\bullet$ of degree k is a pair (d_0, d_+) of a degree k derivation d_+ of the graded Lie algebra $\overline{K}_+$, and of a 1-cocycle $d_0 : \overline{K}_0 \to \overline{K}_k$ which measures the defect of $\overline{K}_0$-equivariance of d_+. Let $\mathrm{Der}_k(\overline{K}_\bullet)$ denote the $\mathbb{Z}$-module of degree k derivations of $\overline{K}_\bullet$. Then, for every $k \geq 1$, the *k-th Johnson homomorphism*

$$\tau_k : \mathcal{G}_k \longrightarrow \mathrm{Der}_k(\overline{K}_\bullet)$$

is defined similarly to (1.5). Specifically, for $f \in \mathcal{G}_k$, the formula

$$\tau_k(f)([x]_i) = \left[f(x)x^{-1} \right]_{i+k} \quad (x \in K_i, i \geq 0),$$

defines a derivation $\tau_k^+(f)$ of $\overline{K}_+$ for $i > 0$ and a 1-cocycle $\tau_k^0(f) : \overline{K}_0 \to \overline{K}_k$ for $i = 0$. The τ_k for $k \geq 1$ form an embedding

$$\overline{\tau}_+ : \overline{\mathcal{G}}_+ \longrightarrow \mathrm{Der}_+(\overline{K}_\bullet) \tag{1.11}$$

of graded Lie algebras. Under a certain formality assumption on the extended N-series K_*, and similarly to (1.10), we also obtain a group embedding

$$\varrho^\theta : \mathcal{G}_1 \longrightarrow \widehat{\mathrm{Der}}_+(\overline{K}_\bullet^{\mathbb{Q}}), \tag{1.12}$$

which induces the rationalization of (1.11) at the graded level.

Group	mapping class group $\mathcal{M}$	handlebody group $\mathcal{H}$
Action	on the group π	on the pair (π, A)
Filtration	$(\mathcal{M}_k)_{k\geq 0}$	$(\mathcal{H}_k)_{k\geq 0}$
0-th graded quotient	$\mathcal{M}_0/\mathcal{M}_1 \simeq \mathrm{Sp}(H)$	$\mathcal{H}_0/\mathcal{H}_1 \simeq \mathrm{Aut}(F)$
1-st subgroup	$\mathcal{M}_1 = \mathcal{I}$, the Torelli group	$\mathcal{H}_1 = \mathcal{T}$, the twist group
Johnson homomorphisms	$\tau_k : \mathcal{M}_k \to \mathrm{Der}_k^\omega\big(\mathrm{Lie}(H)\big)$	$\tau_k : \mathcal{H}_k \to \mathrm{Der}_k^\zeta\big(F \ltimes \mathrm{Lie}(\mathbb{A})\big)$
"Infinitesimal" action	$\varrho^\theta : \mathcal{I} \to \widehat{\mathrm{Der}}_+^\omega\big(\mathrm{Lie}(H^{\mathbb{Q}})\big)$	$\varrho^\theta : \mathcal{T} \to \widehat{\mathrm{Der}}_+^\zeta\big(F \ltimes \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})\big)$
Diagram space	$\mathcal{D}(H^{\mathbb{Q}})$	$\mathcal{D}(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$

TABLE 1. Comparison between the Johnson–Morita theories for the mapping class group and the handlebody group.

1.3. **Johnson–Morita theory for free pairs.** In Section 3, we apply the above constructions to a *free pair* (π, A), a pair of a free group π of finite rank and a non-abelian normal subgroup $\mathsf{A} \leq \pi$ with $F := \pi/\mathsf{A}$ free of finite rank. A free pair (π, A) yields an extended N-series A_*:

$$\mathsf{A}_0 := \pi \quad \text{and} \quad \mathsf{A}_i := \Gamma_i \mathsf{A} \text{ for } i \geq 1.$$

The associated extended graded Lie algebra $\bar{\mathsf{A}}_\bullet$ of A_* consists of the group $\bar{\mathsf{A}}_0 = F$ and the free Lie algebra $\bar{\mathsf{A}}_+ = \mathrm{Lie}(\mathbb{A})$ on the abelianization $\mathbb{A} := \mathsf{A}_{\mathrm{ab}} = \mathsf{A}/\Gamma_2\mathsf{A}$. So, with a slight abuse of notation, we write

$$\bar{\mathsf{A}}_\bullet = F \ltimes \mathrm{Lie}(\mathbb{A}),$$

where the action of F on $\mathbb{A}$ makes $\mathbb{A}$ into a free $\mathbb{Z}[F]$-module of finite rank.

Let

$$\mathcal{G} := \mathrm{Aut}(\pi, \mathsf{A}) = \big\{ f \in \mathrm{Aut}(F) : f(\mathsf{A}) = \mathsf{A} \big\},$$

which acts on the extended N-series A_*. Hence, there is a Johnson filtration $\mathcal{G}_*$ and a family of Johnson homomorphism $(\tau_k)_{k\geq 1}$. By [HM18, §10.1] we have

$$\mathcal{G}_k = \mathcal{G}_k^1 \quad \text{for } k \geq 1, \tag{1.13}$$

see (3.2). Similarly, for $f \in \mathcal{G}_k$, the derivation $\tau_k^+(f)$ determines the 1-cocycle $\tau_k^0(f)$, but the converse may not be true. We also observe that the extended N-series A_* is formal. Hence we get in Theorem 3.7 an embedding (1.12) of $\mathcal{G}_1$ into $\widehat{\mathrm{Der}}_+\big(F \ltimes \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})\big)$.

In Section 4, we construct a map

$$J^F : \mathcal{G} \longrightarrow \mathrm{GL}(p+q; \mathbb{Z}[F]), \tag{1.14}$$

where $q = \mathrm{rank}\, F$ and $p = \mathrm{rank}\, \pi - \mathrm{rank}\, F$, by reducing the coefficients of the Magnus representation of $\mathcal{G} = \mathrm{Aut}(\pi, \mathsf{A})$ to $\mathbb{Z}[F]$. The map J^F factors through $\mathcal{G}/\mathcal{G}_2$ and is our main tool to determine the first terms of the Johnson filtration

$$\mathcal{G} = \mathcal{G}_0 \geq \mathcal{G}_1^0 \geq \mathcal{G}_1 \geq \mathcal{G}_2^0 \geq \cdots .$$

In particular, $\mathcal{G}_1^0/\mathcal{G}_1$ is non-trivial, see Proposition 4.4.

1.4. **Johnson–Morita theory for the handlebody group.** Section 5 gets to the heart of the subject, namely the *handlebody group* $\mathcal{H}$, which is the mapping class group of the handlebody V relative to a disk $D \subset \partial V$. The comparison between the Johnson–Morita theory of the mapping class group and our approach for the handlebody group is sketched in Table 1.

Let $\Sigma := \partial V \setminus \mathrm{int}(D)$, which is a compact, oriented surface with $\partial\Sigma \cong S^1$. Let $g \geq 1$ be the genus of Σ. Let $\iota : \Sigma \to V$ be the inclusion, and let $F := \pi_1(V, \star)$. Then we get a free pair (π, A), where

$$\pi := \pi_1(\Sigma, \star) \quad \text{and} \quad \mathsf{A} := \ker(\iota_* : \pi \longrightarrow F).$$

In the following, we apply the previous constructions to this free pair. The filtrations $(\mathcal{G}_k)_{k\geq 0}$ and $(\mathcal{G}^0_k)_{k\geq 0}$ of $\mathcal{G} = \mathrm{Aut}(\pi, \mathsf{A})$ restrict to filtrations $(\mathcal{H}_k)_{k\geq 0}$ and $(\mathcal{H}^0_k)_{k\geq 0}$ of $\mathcal{H}$, respectively.

Theorem 1.2 (Griffiths [Gri64], see Theorem 5.2)**.** *We have $\mathcal{H} = \mathcal{M} \cap \mathcal{G}$. In other words, a mapping class g of Σ rel $\partial\Sigma$ extends to a mapping class of V rel D if and only if g fixes A setwise.*

By (1.13), we have $\mathcal{H}_k = \mathcal{H}^1_k \subset \mathcal{H}^0_k$ for $k \geq 1$. Using the identity $f(\zeta) = \zeta \in \pi$ for $f \in \mathcal{H}$, we obtain the following, which was announced in [HM18, Ex. 10.9].

Theorem 1.3 (see Theorem 5.3)**.** *We have $\mathcal{H}_k = \mathcal{H}^0_k$ for $k \geq 1$.*

Thus, we may redefine the Johnson filtration of $\mathcal{H}$ as follows.

Corollary 1.4. *We have an extended N-series*

$$\mathcal{H} = \mathcal{H}_0 \geq \mathcal{H}_1 \geq \mathcal{H}_2 \geq \cdots$$

with trivial intersection, satisfying for any $k \geq 1$

$$\mathcal{H}_k = \ker\big(\mathcal{H} \longrightarrow \mathrm{Aut}(\pi/\Gamma_k\mathsf{A})\big) = \ker\big(\mathcal{H} \longrightarrow \mathrm{Aut}(\mathsf{A}/\Gamma_{k+1}\mathsf{A})\big).$$

The first subgroup of the Johnson filtration

$$\mathcal{T} := \mathcal{H}_1 = \ker(\mathcal{H} \longrightarrow \mathrm{Aut}(F))$$

is known as the *twist group* or the *Luft subgroup* of $\mathcal{H}$. Indeed, Luft [Lu78] (see Theorem 5.1) showed that $\mathcal{T}$ is generated by Dehn twists along *meridians* of V, i.e. simple closed curves in Σ bounding properly embedded disks in V.

Section 6 considers the first few terms of the Johnson filtration $(\mathcal{H}_k)_{k\geq 1}$. Since the canonical homomorphism $\mathcal{H} \to \mathrm{Aut}(F)$ is surjective, we have an isomorphism

$$\mathcal{H}/\mathcal{T} = \mathcal{H}_0/\mathcal{H}_1 \simeq \mathrm{Aut}(F).$$

Furthermore, a homomorphism $\mathrm{Mag} : \mathcal{T} \to \mathrm{Mat}(g \times g; \mathbb{Z}[F])$ extracted from (1.14) embeds $\mathcal{H}_1/\mathcal{H}_2$ into a space of hermitian matrices, see Proposition 6.2.

In Section 7, we consider the Johnson homomorphisms for the handlebody group. While τ_1 is equivalent to the above representation $\mathrm{Mag} : \mathcal{T} \to \mathrm{Mat}(g \times g; \mathbb{Z}[F])$, we need a more general approach to study the Johnson homomorphisms in arbitrary degrees. They form a morphism of graded Lie algebras

$$\overline{\tau}_+ : \overline{\mathcal{H}}_+ \longrightarrow \mathrm{Der}^\zeta_+\big(F \ltimes \mathrm{Lie}(\mathbb{A})\big), \tag{1.15}$$

whose source is the associated graded of the Johnson filtration, and whose target consists of positive-degree derivations of $\overline{\mathsf{A}}_\bullet$ that vanish on the boundary element $[\zeta]_1 \in \overline{\mathsf{A}}_1 = \mathbb{A}$. We call $\mathrm{Der}^\zeta_+\big(F \ltimes \mathrm{Lie}(\mathbb{A})\big)$ the *Lie algebra of special derivations*, which is the analogue of the Lie algebra of symplectic derivations in the handlebody case. We also refine formality of the free pair (π, A) with the boundary condition (see Lemma 7.3): this leads to *special expansions* of (π, A), which should be compared to symplectic expansions of π. Thus, we obtain the following analogue of (1.10) for the handlebody group.

Theorem 1.5 (see Theorem 7.4)**.** *Let θ be a special expansion of (π, A). There is an embedding*

$$\varrho^{\theta} : \mathcal{T} \longrightarrow \widehat{\mathrm{Der}}^{\zeta}_{+}\big(F \ltimes \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})\big) \tag{1.16}$$

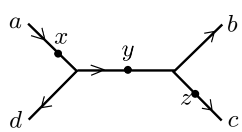
of the twist group into the degree-completed Lie algebra of special derivations (equipped with the BCH product), which induces (1.15) *on the associated graded (with rational coefficients)*

In Section 8, we consider the canonical maps $\mathrm{Der}_{+}(F \ltimes \mathrm{Lie}(\mathbb{A})) \to Z^1(F, \mathrm{Lie}(\mathbb{A}))$ and $\mathrm{Der}_{+}(F \ltimes \mathrm{Lie}(\mathbb{A})) \to \mathrm{Hom}(\mathbb{A}, \mathrm{Lie}(\mathbb{A}))$ which associate to any derivation $d = (d_0, d_+)$ the corresponding 1-cocycle d_0 and the restriction $d_+|_{\mathbb{A}}$ of the corresponding derivation, respectively. Let

$$D^0_+ \subset Z^1(F, \mathrm{Lie}(\mathbb{A})) \quad \text{and} \quad D^1_+ \subset \mathrm{Hom}(\mathbb{A}, \mathrm{Lie}(\mathbb{A}))$$

be the subgroups defined by the boundary condition $d([\zeta]_1) = 0$, which is satisfied by any $d \in \mathrm{Der}^{\zeta}_{+}(F \ltimes \mathrm{Lie}(\mathbb{A}))$. It turns out that the corresponding homomorphisms $\mathrm{Der}^{\zeta}_{+}(F \ltimes \mathrm{Lie}(\mathbb{A})) \to D^0_+$ and $\mathrm{Der}^{\zeta}_{+}(F \ltimes \mathrm{Lie}(\mathbb{A})) \to D^1_+$ are isomorphisms. Thus, we obtain two descriptions D^0_+ and D^1_+ of the Lie algebra $\mathrm{Der}^{\zeta}_{+}(F \ltimes \mathrm{Lie}(\mathbb{A}))$, and we are free to work with either the 1-cocycles $\tau^0_k(f) \in D^0_k$ or the homomorphisms $\tau^1_k(f) \in D^1_k$ for $f \in \mathcal{H}_k$.

We give in Section 9 a diagrammatic description of the graded Lie algebra $\mathrm{Der}^{\zeta}_{+}(F \ltimes \mathrm{Lie}(\mathbb{A}))$ with rational coefficients. Specifically, we consider a $\mathbb{Q}$-vector space $\mathcal{D}(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$ that is generated by oriented trivalent trees with leaves colored by $\mathbb{A}^{\mathbb{Q}} := \mathbb{A} \otimes \mathbb{Q}$ and edges colored by $\mathbb{Q}[F]$. For example, here is a generator in degree 3:



(with $a, b, c, d \in \mathbb{A}^{\mathbb{Q}}$ and $x, y, z \in \mathbb{Q}[F]$)

In comparison with the space $\mathcal{D}(H^{\mathbb{Q}})$ which serves for the mapping class group of Σ, the definition of $\mathcal{D}(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$ involves the cocommutative Hopf algebra $\mathbb{Q}[F]$ and the $\mathbb{Q}[F]$-module $\mathbb{A}^{\mathbb{Q}}$. We obtain the following analogue of (1.8) for the handlebody group.

Theorem 1.6 (See Theorem 9.7)**.** *There is a graded Lie $\mathbb{Q}$-algebra isomorphism*

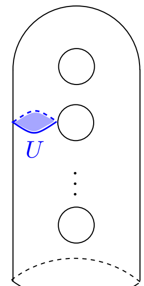
$$\mathrm{Der}^{\zeta}_{+}\big(F \ltimes \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})\big) \simeq \mathcal{D}\big(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F]\big),$$

where the Lie bracket of trees is defined by "grafting leaves-to-beads" and "branching leaves-to-leaves" using intersection operations $\Theta : \mathbb{Z}[F] \times \mathbb{A} \to \mathbb{Z}[F] \otimes \mathbb{Z}[F]$ and $\Psi : \mathbb{A} \times \mathbb{A} \to \mathbb{Z}[F] \otimes \mathbb{A}$, respectively.

Thus, the Lie bracket in $\mathcal{D}(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$ is an analogue of (1.9), where the operations Θ and Ψ play the role of the pairing ω. These operations, presented in Appendix A, are derived from the "homotopy intersection form" η of Σ [Tu78]. The properties of Θ and Ψ necessary for the proof of Theorem 9.7 are derived from the axioms of a "quasi-Poisson double bracket", which is produced from η [MT14].

Section 10 is devoted to explicit computations of the Johnson homomorphisms, starting with the degree 1 case:

Example 1.7. Consider the first Johnson homomorphism $\tau_1^0 : \mathcal{H}_1 \to D_1^0$, defined on the twist group $\mathcal{H}_1 = \mathcal{T}$. We can identify the target D_1^0 with $\mathrm{Sym}^2(\mathbb{A})_{\mathbb{Z}[F]}$, the $\mathbb{Z}[F]$-coinvariants of the symmetric tensors $\mathrm{Sym}^2(\mathbb{A})$. For any properly embedded disk $U \subset V$, we have



$$\tau_1^0\big(T_{\partial U}\big) = -[u] \otimes [u] \in D_1^0, \tag{1.17}$$

where $u \in \mathsf{A}$ is obtained from the closed curve ∂U by orienting it and basing it at $\star$ in an arbitrary way (see Proposition 10.1).

Using the diagrammatic formula for the Lie bracket in $\mathrm{Der}_+^\zeta\big(F \ltimes \mathrm{Lie}(\mathbb{A}^\mathbb{Q})\big) \simeq \mathcal{D}(\mathbb{A}^\mathbb{Q}, \mathbb{Q}[F])$, one can use (1.17) to compute τ_k on $\Gamma_k\mathcal{T} \subset \mathcal{H}_k$. Furthermore, (1.17) is the key to a new proof of the following:

Theorem 1.8 (McCullough [Mc84], see Theorem 10.3)**.** *The abelianization of $\mathcal{T}$ surjects onto a free abelian group of countably-infinite rank, so it is not finitely generated.*

Next, as a strong generalization of (1.17), we compute the representation (1.16) on a Dehn twist $T_{\partial U}$ along an arbitrary meridian ∂U, and for any special expansion θ of the free pair (π, A) (Theorem 10.5). This is an analogue of a formula of Kawazumi and Kuno [KK14], who computed (1.10) for an arbitrary Dehn twist.

Finally, we consider embeddings of the pure braid group PB_g into the twist group $\mathcal{T}$. Theorem 10.9 relates the lower central series of PB_g to the Johnson filtration of $\mathcal{H}$ and, consequently, Milnor invariants to Johnson homomorphisms. (An analogous result for the surface mapping class groups was given by Gervais and Habegger [GH02].) In particular, this illustrates the non-triviality of the Johnson–Morita theory for $\mathcal{H}$ in any degrees.

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Conventions. Unless otherwise stated, all group actions are *left* actions and modules (over any ring) are *left* modules. If a group G acts on an abelian group A, then the action of $g \in G$ on $a \in A$ is denoted by ${}^g a$ or $g \cdot a$, or even ga if there is no risk of confusion. If not specified, the ground ring for linear algebra is $\mathbb{Z}$.

If S is a subset of a group G, let $\langle S \rangle$ denote the subgroup of G generated by S, and $\langle\!\langle S \rangle\!\rangle$ the subgroup normally generated by S. For all $x, y \in G$, we set ${}^x y = xyx^{-1}$, $y^x = x^{-1}yx$ and $[x, y] = xyx^{-1}y^{-1}$. For any two subgroups K, H of G, let $[K, H]$ denote the subgroup of G generated by the commutators $[k, h]$ for $k \in K, h \in H$.

For any two $\mathbb{Z}$-modules U and V, an element $z \in U \otimes V$ is sometimes denoted by $z^\ell \otimes z^r$ to suggest its expansion $z = \sum_i u_i \otimes v_i$ in terms of finitely many elements $u_i \in U$ and $v_i \in V$.

2. Johnson homomorphisms for an extended N-series

In this section, we summarize parts of the theory of generalized Johnson homomorphisms as developed in [HM18] for extended N-series.

2.1. Extended N-series and extended graded Lie algebras.

An *extended N-series* $K_* = (K_m)_{m\geq 0}$ is a descending series of subgroups

$$K_0 \geq K_1 \geq \cdots \geq K_k \geq \cdots$$

such that $[K_m, K_n] \leq K_{m+n}$ for all $m, n \geq 0$. In particular, K_m is normal in K_0 for any $m \geq 0$. An *automorphism* of K_* is an automorphism f of K_0 with $f(K_m) = K_m$ for all $m \geq 0$. Let $\mathrm{Aut}(K_*)$ denote the group of all automorphisms of K_*.

An *extended graded Lie algebra* $L_\bullet = (L_m)_{m\geq 0}$ consists of a group L_0, a graded Lie algebra $L_+ = (L_m)_{m\geq 1}$ and an action $(z, x) \mapsto {}^z x$ of L_0 on L_+ by graded Lie algebra automorphisms. Any extended N-series K_* has an *associated* extended graded Lie algebra $\overline{K}_\bullet$ defined by $\overline{K}_m = K_m/K_{m+1}$ for all $m \geq 0$, where the Lie bracket in $\overline{K}_\bullet$ is induced by the commutator operation $(x, y) \mapsto [x, y]$, and $\overline{K}_0$ acts on $\overline{K}_+$ by conjugation $(x, y) \mapsto {}^x y$.

We will sometimes need the rational version $\overline{K}_\bullet^{\mathbb{Q}}$ defined by $\overline{K}_0^{\mathbb{Q}} = K_0/K_1$ and the graded Lie $\mathbb{Q}$-algebra $\overline{K}_+^{\mathbb{Q}} = \big((K_m/K_{m+1}) \otimes \mathbb{Q}\big)_{m\geq 1}$.

A *morphism* $f_\bullet = (f_m)_{m\geq 0} : L_\bullet \to L'_\bullet$ of extended graded Lie algebras consists of a group homomorphism $f_0 : L_0 \to L'_0$, and a graded Lie algebra homomorphism $f_+ = (f_m)_{m\geq 1} : L_+ \to L'_+$ which is equivariant over f_0:

$$f_m({}^x y) = {}^{f_0(x)}(f_m(y)) \quad \text{for all } x \in L_0,\ y \in L_m,\ m \geq 1.$$

A *derivation* of *degree* $m \geq 1$ of an extended graded Lie algebra $L_\bullet$ is a family $d = (d_i)_{i\geq 0}$ of maps $d_i : L_i \to L_{m+i}$ satisfying the following conditions.

(1) $d_+ = (d_i)_{i\geq 1}$ is a derivation of the graded Lie algebra L_+, i.e.

$$d_{i+j}([a, b]) = [d_i(a), b] + [a, d_j(b)] \quad \text{for all } a \in L_i,\ b \in L_j,\ i, j \geq 1.$$

(2) $d_0 : L_0 \to L_m$ is a 1-cocycle, i.e.

$$d_0(ab) = d_0(a) + {}^a(d_0(b)) \quad \text{for all } a, b \in L_0.$$

(3) d_0 controls the defect of L_0-equivariance of d_+, i.e.

$$d_i({}^a b) = {}^a(d_i(b)) + [d_0(a), {}^a b] \quad \text{for all } a \in L_0,\ b \in L_i,\ i \geq 1.$$

Let $\mathrm{Der}_m(L_\bullet)$ be the set of derivations of $L_\bullet$ of degree m. Then $\mathrm{Der}_+(L_\bullet) := (\mathrm{Der}_m(L_\bullet))_{m\geq 1}$ is a graded Lie algebra whose Lie bracket generalizes the usual Lie bracket for derivations of L_+ [HM18, Theorem 5.2]. Furthermore, $\mathrm{Der}_0(L_\bullet) := \mathrm{Aut}(L_\bullet)$ acts on $\mathrm{Der}_+(L_\bullet)$ by conjugation and we get an extended graded Lie algebra $\mathrm{Der}_\bullet(L_\bullet)$ [HM18, Theorem 5.3]. The necessary definitions will appear in Section 3.

Let K_* be an extended N-series. An *action* of a group $\mathcal{G}$ on K_* is an action of $\mathcal{G}$ on K_0 such that $g(K_m) = K_m$ for all $g \in \mathcal{G}, m \geq 0$. In other words, it is a homomorphism $\mathcal{G} \to \mathrm{Aut}(K_*)$. In this case, K_* induces an extended N-series $\mathcal{G}_*$, called the *Johnson filtration* and defined by

$$\mathcal{G}_m := \bigcap_{j\geq 0} \mathcal{G}_m^j, \quad \text{where } \mathcal{G}_m^j := \big\{ g \in \mathcal{G} \mid g(x)x^{-1} \in K_{m+j} \text{ for all } x \in K_j \big\} \tag{2.1}$$

for $m \geq 0$. Note that $\mathcal{G}_0 = \mathcal{G}$. There is an injective extended graded Lie algebra morphism

$$\bar{\tau}_\bullet : \overline{\mathcal{G}}_\bullet \longrightarrow \mathrm{Der}_\bullet(\overline{K}_\bullet), \tag{2.2}$$

called the *Johnson morphism*. For the definition of $\bar{\tau}_\bullet$, see [HM18, §6] and also Section 3.

Remark 2.1. The study of extended N-series includes that of *N-series*, which were considered in full generality by Darné, too [Dar19]. (Indeed, an N-series is an extended N-series K_* for which the acting group K_0/K_1 is trivial.)

2.2. **Formal extended N-series.** For now, we work over $\mathbb{Q}$. If K_* is formal in some sense, then the graded Lie algebra homomorphism $\bar{\tau}_+$ in (2.2) is the associated graded of an "infinitesimal" action of $\mathcal{G}$ on K_*. We review below such a situation, and refer the reader to [SW19, SW20] for a general introduction to formality of groups.

The extended N-series K_* induces a filtration $J^{\mathbb{Q}}_*(K_*)$ of the algebra $\mathbb{Q}[K_0]$, where $J^{\mathbb{Q}}_m(K_*)$ is the ideal generated by the elements of the form $(x_1-1)\cdots(x_p-1)$ for all $x_1 \in K_{m_1}, \dots, x_p \in K_{m_p}$, $m_1+\cdots+m_p \geq m$, $m_1,\dots,m_p \geq 1$, $p \geq 1$. Then the Hopf algebra structure of $\mathbb{Q}[K_0]$ is compatible with the filtration $J^{\mathbb{Q}}_*(K_*)$. Therefore we have a graded Hopf $\mathbb{Q}$-algebra

$$\mathrm{gr}_\bullet\big(J^{\mathbb{Q}}_*(K_*)\big) = \bigoplus_{i\geq 0} J^{\mathbb{Q}}_i(K_*)/J^{\mathbb{Q}}_{i+1}(K_*)$$

and a complete Hopf $\mathbb{Q}$-algebra

$$\widehat{\mathbb{Q}[K_*]} = \varprojlim_k \ \mathbb{Q}[K_0]\,/J^{\mathbb{Q}}_k(K_*).$$

The extended N-series K_* is said to be *formal* if $\widehat{\mathbb{Q}[K_*]}$ is isomorphic to the degree-completion of $\mathrm{gr}_\bullet\big(J^{\mathbb{Q}}_*(K_*)\big)$ through an isomorphism whose associated graded is the identity.

We can characterize the formality as follows. First of all, we have the following generalization for extended N-series [HM18, Theorem 11.2] of a classical result of Quillen for the lower central series of groups [Qui68]:

$$\mathrm{gr}_\bullet\big(J^{\mathbb{Q}}_*(K_*)\big) \simeq U(\overline{K}^{\mathbb{Q}}_\bullet). \tag{2.3}$$

Here $U(\overline{K}^{\mathbb{Q}}_\bullet)$ is the *universal enveloping algebra* of the extended graded Lie $\mathbb{Q}$-algebra $\overline{K}^{\mathbb{Q}}_\bullet$. As a $\mathbb{Q}$-coalgebra, $U(\overline{K}^{\mathbb{Q}}_\bullet)$ is the tensor product $U(\overline{K}^{\mathbb{Q}}_+)\otimes_{\mathbb{Q}}\mathbb{Q}[K_0/K_1]$ of the usual universal enveloping algebra of the Lie $\mathbb{Q}$-algebra $\overline{K}^{\mathbb{Q}}_+$ and the group algebra of K_0/K_1. The multiplication is defined by

$$(v\otimes y)\cdot(v'\otimes y') = v\,{}^{y}v'\otimes yy' \quad \text{for all } v,v' \in U(\overline{K}^{\mathbb{Q}}_+) \text{ and } y,y' \in K_0/K_1. \tag{2.4}$$

We regard $U(\overline{K}^{\mathbb{Q}}_+)$ and $\mathbb{Q}[K_0/K_1]$ as subalgebras of $U(\overline{K}^{\mathbb{Q}}_\bullet)$ in the obvious way, and any element $v\otimes y \in U(\overline{K}^{\mathbb{Q}}_+)$ is written as a product $v\cdot y$, see [HM18, §11] for details. The extended N-series K_* is formal if and only if there is a monoid homomorphism

$$\theta : K_0 \longrightarrow \hat{U}(\overline{K}^{\mathbb{Q}}_\bullet)$$

which takes values in the degree-completion $\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})$ of $U(\overline{K}_{\bullet}^{\mathbb{Q}})$ and maps any $x \in K_i$ $(i \geq 0)$ to a group-like element of the form

$$\theta(x) = \begin{cases} 1 + [x]_i + (\deg > i) & \text{if } i > 0, \\ [x]_0 + (\deg > 0) & \text{if } i = 0, \end{cases} \tag{2.5}$$

where $[x]_i$ denotes the class of x modulo K_{i+1}.

In such a case, θ is called an *expansion* of the extended N-series K_* and it allows for the following constructions. Consider the homomorphism

$$\rho^\theta : \mathcal{G} \longrightarrow \operatorname{Aut}\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big), \quad g \longmapsto \hat{\theta} \circ \widehat{\mathbb{Q}[g]} \circ \hat{\theta}^{-1},$$

where $\widehat{\mathbb{Q}[g]}$ denotes the automorphism of $\widehat{\mathbb{Q}[K_*]}$ induced by the action of g on K_0 and the isomorphism $\hat{\theta} : \widehat{\mathbb{Q}[K_*]} \to \hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})$ is the extension of θ. Note that ρ^θ takes values in the group $\operatorname{IAut}\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big)$ of complete Hopf algebra automorphisms of $\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})$ that induce the identity on the associated graded. Let also

$$\operatorname{Der}_+\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big)$$

be the space of derivations of the algebra $\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})$ that map every $x \in \overline{K}_0^{\mathbb{Q}} = K_0/K_1$ to $\widehat{\overline{K}}_+^{\mathbb{Q}} x$ and that maps $\widehat{\overline{K}}_{\geq m}^{\mathbb{Q}}$ to $\widehat{\overline{K}}_{\geq m+1}^{\mathbb{Q}}$ for every $m \geq 1$. According to the following lemma, which is implicit in [HM18, §12], there is a one-to-one correspondence between positive-degree derivations of the extended graded Lie $\mathbb{Q}$-algebra $\overline{K}_{\bullet}^{\mathbb{Q}}$ and derivations of its universal enveloping algebra of the previous type.

Lemma 2.2. *There are canonical $\mathbb{Q}$-linear isomorphisms*

$$\operatorname{IAut}\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big) \xrightarrow[\simeq]{\log} \operatorname{Der}_+\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big) \xrightarrow[\simeq]{\text{res}} \widehat{\operatorname{Der}}_+(\overline{K}_{\bullet}^{\mathbb{Q}}).$$

Here $\log$ *is the formal logarithm series, i.e. it maps any automorphism a to*

$$\log(a) := \sum_{n \geq 1} \frac{(-1)^{n+1}}{n!} (a - \mathrm{id})^n,$$

and res *is the restriction map, which maps any derivation d to*

$$\operatorname{res}(d) := (d_0, d_+) \quad \textit{where} \quad d_0(x) = d(x)x^{-1},\ x \in \overline{K}_0 \quad \textit{and} \quad d_+(u) = d(u),\ u \in \overline{K}_+^{\mathbb{Q}}.$$

Proof. The map $\log : \operatorname{IAut}\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big) \to \operatorname{Der}_+\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big)$ is proved to be well-defined by following the first four paragraphs of the proof of [HM18, Lemma 12.5].

To construct the inverse to log, observe that any $d \in \operatorname{Der}_+\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big)$ increases degrees, hence the formal power series

$$\exp(d) := \sum_{n \geq 1} \frac{d^n}{n!}$$

converges and induces the identity on the associated graded. Since d is an algebra derivation, $\exp(d)$ is an algebra automorphism. Besides, d is a coderivation, i.e. we have the identity $\Delta d = (d \hat{\otimes} \mathrm{id} + \mathrm{id} \hat{\otimes} d)\Delta$, as can be checked on the elements of $\overline{K}_{\bullet}^{\mathbb{Q}}$ (which generate the algebra $U(\overline{K}_{\bullet}^{\mathbb{Q}})$). Therefore $\exp(d)$ is a coalgebra map. Thus, we obtain a map $\exp : \operatorname{Der}_+\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big) \to \operatorname{IAut}\big(\hat{U}(\overline{K}_{\bullet}^{\mathbb{Q}})\big)$, which is inverse to log.

The map $\mathrm{res} : \mathrm{Der}_+\big(\hat U(\overline{K}^{\mathbb{Q}}_\bullet)\big) \to \widehat{\mathrm{Der}}_+(\overline{K}^{\mathbb{Q}}_\bullet)$ is proved to be well-defined by following the last paragraph of the proof of [HM18, Lemma 12.5]. Since $\overline{K}^{\mathbb{Q}}_\bullet$ generate the algebra $U(\overline{K}^{\mathbb{Q}}_\bullet)$, this map is injective.

To show that res is also surjective, let $(d_0, d_+) \in \widehat{\mathrm{Der}}_+(\overline{K}^{\mathbb{Q}}_\bullet)$. The Lie algebra derivation d_+ of $\overline{K}^{\mathbb{Q}}_+$ extends to a unique algebra derivation $\tilde d_+$ of its universal enveloping algebra. Besides, let $\tilde d_0 : \mathbb{Q}[K_0/K_1] \to \hat U(\overline{K}^{\mathbb{Q}}_\bullet)$ be the $\mathbb{Q}$-linear map defined by $\tilde d_0(x) = d_0(x)x$ for any $x \in K_0/K_1$. Then, there is a unique $\mathbb{Q}$-linear map $\tilde d : U(\overline{K}^{\mathbb{Q}}_\bullet) \to \hat U(\overline{K}^{\mathbb{Q}}_\bullet)$ defined by $\tilde d(vy) = \tilde d_+(v)\, y + v\, \tilde d_0(y)$ for any $v \in U(\overline{K}^{\mathbb{Q}}_+)$ and $y \in \mathbb{Q}[K_0/K_1]$. Since $\tilde d$ increases degrees, it extends to $\tilde d : \hat U(\overline{K}^{\mathbb{Q}}_\bullet) \to \hat U(\overline{K}^{\mathbb{Q}}_\bullet)$ by continuity. It remains to check that $\tilde d$ is an algebra derivation. For any $v, v' \in U(\overline{K}^{\mathbb{Q}}_+)$ and $y, y' \in K_0/K_1$, we have

$$\begin{aligned} \tilde d\big((vy)(v'y')\big) &= \tilde d\big((v\, {}^y v')(yy')\big) \\ &= \tilde d_+\big(v\, {}^y v'\big)\, (yy') + (v\, {}^y v')\, \tilde d_0(yy') \\ &= \big(\tilde d_+(v)\, {}^y v' + v\, \tilde d_+({}^y v') + v\, {}^y v'\, d_0(y) + v\, {}^y v'\, {}^y d_0(y')\big) yy' \end{aligned}$$

and, since the defect of $\mathbb{Q}[K_0/K_1]$-equivariance of d_+ (and, so, $\tilde d_+$) is controlled by the 1-cocycle d_0, we get

$$\tilde d\big((vy)(v'y')\big) = \big(\tilde d_+(v)\, {}^y v' + v\, {}^y \tilde d_+(v') + v\, d_0(y)\, {}^y v' + v\, {}^y v'\, {}^y d_0(y')\big)\, yy'.$$

On the other hand, we have

$$(vy)\, \tilde d(v'y') = (vy)\, \big(\tilde d_+(v')\, y' + v'\, \tilde d_0(y')\big) = v\, y\, \tilde d_+(v')\, y' + v\, y\, v' d_0(y') y'$$

and

$$\tilde d(vy)\, (v'y') = \big(\tilde d_+(v)\, y + v\, \tilde d_0(y)\big)\, (v'y') = \tilde d_+(v)\, y\, v'\, y' + v\, d_0(y)\, y\, v'\, y'.$$

We conclude that $\tilde d\big((vy)(v'y')\big) = (vy)\, \tilde d(v'y') + \tilde d(vy)\, (v'y')$. □

The previous lemma shows that, for any $m \geq 1$ and $g \in \mathcal{G}_m$, the automorphism $\rho^\theta(g)$ induces an element $\varrho^\theta(g) \in \widehat{\mathrm{Der}}_+(\overline{K}^{\mathbb{Q}}_\bullet)$ of degree $\geq m$. The complete Lie algebra $\widehat{\mathrm{Der}}_+(\overline{K}^{\mathbb{Q}}_\bullet)$ can be regarded as a filtered group whose multiplication law is defined by the BCH formula. Then we obtain a filtered group homomorphism

$$\varrho^\theta : \mathcal{G}_1 \longrightarrow \widehat{\mathrm{Der}}_+(\overline{K}^{\mathbb{Q}}_\bullet) \tag{2.6}$$

inducing the rational version $\bar\tau^{\mathbb{Q}}_+$ of $\bar\tau_+$ on the associated graded, see [HM18, Theorem 12.6]. We view (2.6) as an infinitesimal version of the action of the group $\mathcal{G}_1$ on the extended N-series K_*.

3. Johnson homomorphisms for a free pair

We continue the review of generalized Johnson homomorphisms by focusing on the automorphism group of a free pair, as in [HM18, §10.1]. We also establish the formality in this case.

3.1. **Free pairs and their automorphism groups.** A *free pair* is a pair (π, A) of a free group π and a non-abelian normal subgroup A with $F := \pi/\mathsf{A}$ free. Let $\varpi : \pi \to F$ denote the canonical projection. In the sequel, for simplicity, we assume that the free groups π and F have finite rank.

Remark 3.1. By [FJ50, Theorem 6.4], π is the free product $A * B$ of subgroups $A, B \leq \pi$ such that $A \subset \mathsf{A}$ and ϖ maps B isomorphically onto F. Thus, there is a basis of π

$$\{\alpha_i\}_{i\in I} \sqcup \{\beta_j\}_{j\in J} \tag{3.1}$$

(with I and J finite) such that $A = \langle \alpha_i \,|\, i\rangle$, $B = \langle \beta_j \,|\, j\rangle$ and $\mathsf{A} = \langle\!\langle \alpha_i \,|\, i\rangle\!\rangle$. Although the constructions in this section are independent of the choices of A, B and their bases, we sometimes use these bases.

An *automorphism* of (π, A) is an automorphism g of π with $g(\mathsf{A}) = \mathsf{A}$. Let $\mathrm{Aut}(\pi, \mathsf{A})$ denote the group of automorphisms of (π, A). Following [HM18, §10.1], let us review how the theory of generalized Johnson homomorphisms applies to $\mathrm{Aut}(\pi, \mathsf{A})$. Let

$$\mathsf{A} = \Gamma_1\mathsf{A} \geq \Gamma_2\mathsf{A} \geq \Gamma_3\mathsf{A} \geq \cdots$$

be the *lower central series* of A, defined inductively by $\Gamma_1\mathsf{A} := \mathsf{A}$ and $\Gamma_{i+1}\mathsf{A} := [\Gamma_i\mathsf{A}, \mathsf{A}]$ $(i \geq 1)$. Setting $\mathsf{A}_0 := \pi$ and $\mathsf{A}_m := \Gamma_m\mathsf{A}$ for $m \geq 1$, we get an extended N-series

$$\mathsf{A}_* := (\mathsf{A}_i)_{i\geq 0},$$

and consequently an extended graded Lie algebra

$$\overline{\mathsf{A}}_\bullet := (\mathsf{A}_m/\mathsf{A}_{m+1})_{m\geq 0}.$$

Lemma 3.2. *The group $\mathbb{A} := \overline{\mathsf{A}}_1 = \mathsf{A}/[\mathsf{A}, \mathsf{A}]$ is free as a $\mathbb{Z}[F]$-module, where the action of F on $\mathbb{A}$ is induced by the conjugation of π on A.*

Proof. Consider a basis of π of type (3.1), and let $[\alpha_i] \in \mathsf{A}/[\mathsf{A}, \mathsf{A}]$ denote the class of $\alpha_i \in \mathsf{A}$. Then the $\mathbb{Z}[F]$-module $\mathbb{A}$ is free on the subset $\big\{[\alpha_i]\big\}_{i\in I}$. □

Since A is a free group, its associated graded $\overline{\mathsf{A}}_+$ is the free Lie algebra $\mathrm{Lie}(\mathbb{A})$ on $\mathbb{A}$. For any $x \in \pi$ and $m \geq 0$, let $[x]_m$ (or sometimes $[x]$) denote the class of x modulo A_{m+1}. Note that if $x \in \mathsf{A}_m$, then $[x]_m \in \overline{\mathsf{A}}_m$.

The group $\mathcal{G} := \mathrm{Aut}(\pi, \mathsf{A})$ acts on the extended N-series A_*. Let $\mathcal{G}_* = (\mathcal{G}_i)_{i\geq 0}$ be the corresponding Johnson filtration, as defined by (2.1). It follows from [HM18, Proposition 10.1] that

$$\mathcal{G}_m = \mathcal{G}_m^0 \cap \mathcal{G}_m^1 \quad \text{for all } m \geq 0,$$

where

$$\mathcal{G}_m^0 = \ker\big(\mathcal{G} \longrightarrow \mathrm{Aut}(\pi/\mathsf{A}_m)\big) \quad \text{and} \quad \mathcal{G}_m^1 = \ker\big(\mathcal{G} \longrightarrow \mathrm{Aut}(\mathsf{A}/\mathsf{A}_{m+1})\big).$$

Furthermore, it follows from [HM18, Theorem 10.2][1] and Lemma 3.2 that

$$\mathcal{G}_m = \mathcal{G}_m^1 \quad \text{for all } m \geq 0. \tag{3.2}$$

[1]The result [HM18, Theorem 10.2] applies to an extended N-series $K_* = (K_m)_{m\geq 0}$ such that $K_m = \Gamma_m K_1$ and K_1 is a non-abelian free group. Its proof is by induction on $m \geq 0$, which is achieved thanks to [HM18, Lemma 10.3]. But, this lemma does not apply for $m = 1$. This gap in [HM18, Theorem 10.2] is fixed by assuming that $\overline{K}_1$ is torsion-free as a $\mathbb{Z}[\overline{K}_0]$-module.

Hence we have two mutually nested filtrations $\mathcal{G}_*$ and $\mathcal{G}^0_*$:

$$\mathcal{G} = \mathcal{G}^0_0 = \mathcal{G}_0 \geq \mathcal{G}^0_1 \geq \mathcal{G}_1 \geq \cdots \geq \mathcal{G}_{m-1} \geq \mathcal{G}^0_m \geq \mathcal{G}_m \geq \cdots . \tag{3.3}$$

Since A is free, we have $\bigcap_i \Gamma_i \mathsf{A} = \{1\}$. Hence

$$\bigcap_{m\geq 0} \mathcal{G}^0_m = \bigcap_{m\geq 0} \mathcal{G}_m = \{1\}. \tag{3.4}$$

3.2. **Truncations of the Johnson morphism for a free pair.** Since the graded Lie algebra $\overline{\mathsf{A}}_+ = \mathrm{Lie}(\mathbb{A})$ is free on its degree 1 part $\mathbb{A}$, any derivation of the extended graded Lie algebra $\overline{\mathsf{A}}_\bullet$ is equivalent to its truncations to the degree 0 and 1 parts of $\overline{\mathsf{A}}_\bullet$. Specifically, there is an isomorphism

$$\mathrm{Der}_m(\overline{\mathsf{A}}_\bullet) \longrightarrow D_m(\overline{\mathsf{A}}_\bullet), \quad (d_i)_{i\geq 0} \longmapsto (d_0, d_1), \tag{3.5}$$

where

$$\begin{aligned} D_0(\overline{\mathsf{A}}_\bullet) \;&=\; \big\{(d_0,d_1) \in \mathrm{Aut}(F) \times \mathrm{Aut}(\mathbb{A}) \\ &\qquad \big| \; d_1({}^f a) = {}^{d_0(f)}(d_1(a)) \text{ for } f \in F,\ a \in \mathbb{A}\big\} \end{aligned} \tag{3.6}$$

and, for every $m \geq 1$,

$$\begin{aligned} D_m(\overline{\mathsf{A}}_\bullet) \;&=\; \big\{(d_0,d_1) \in Z^1(F,\overline{\mathsf{A}}_m) \times \mathrm{Hom}(\mathbb{A},\overline{\mathsf{A}}_{m+1}) \\ &\qquad \big| \; d_1({}^f a) = [d_0(f), {}^f a] + {}^f(d_1(a)) \text{ for } f \in F, a \in \mathbb{A}\big\}. \end{aligned} \tag{3.7}$$

According to [HM18, Proposition 7.4], the extended graded Lie algebra structure on $\mathrm{Der}_\bullet(\overline{\mathsf{A}}_\bullet)$ corresponds through (3.5) to the following extended graded Lie algebra structure on $D_\bullet(\overline{\mathsf{A}}_\bullet)$:

- the Lie bracket $[d,e] \in D_{m+n}(\overline{\mathsf{A}}_\bullet)$ of $d = (d_0,d_1) \in D_m(\overline{\mathsf{A}}_\bullet)$ and $e = (e_0,e_1) \in D_n(\overline{\mathsf{A}}_\bullet)$ with $m,n \geq 1$ is defined by

$$[d,e]_0(f) = d_n(e_0(f)) - e_m(d_0(f)) - [d_0(f), e_0(f)] \quad \text{for } f \in F, \tag{3.8}$$

$$[d,e]_1(a) = d_{n+1}(e_1(a)) - e_{m+1}(d_1(a)) \quad \text{for } a \in \mathbb{A}, \tag{3.9}$$

  where $d_+ = (d_i)_{i\geq 1}$ and $e_+ = (e_j)_{j\geq 1}$ are the derivations of $\overline{\mathsf{A}}_+$ extending d_1 and e_1, respectively;
- the action ${}^e d \in D_m(\overline{\mathsf{A}}_\bullet)$ of $e = (e_0,e_1) \in D_0(\overline{\mathsf{A}}_\bullet)$ on $d = (d_0,d_1) \in D_m(\overline{\mathsf{A}}_\bullet)$ with $m \geq 1$ is defined by

$$({}^e d)_0(f) \;=\; e_m d_0 e_0^{-1}(f) \quad \text{for } f \in F, \tag{3.10}$$

$$({}^e d)_1(a) \;=\; e_{m+1} d_1 e_1^{-1}(a) \quad \text{for } a \in \mathbb{A}, \tag{3.11}$$

  where $e_+ = (e_i)_{i\geq 1}$ is the automorphism of $\overline{\mathsf{A}}_+$ extending e_1.

We now apply the truncation isomorphism (3.5) to the Johnson morphism $\bar{\tau}_\bullet$ mentioned in (2.2). For every $m \geq 0$, let τ^0_m and τ^1_m denote the two components of the image of $\bar{\tau}_m$ in $\mathrm{Der}_m(\overline{\mathsf{A}}_\bullet)$ by the map (3.5). Hence, for $m = 0$, we get two homomorphisms

$$\tau^0_0 : \mathcal{G}_0 \longrightarrow \mathrm{Aut}(F) \quad \text{and} \quad \tau^1_0 : \mathcal{G}_0 \longrightarrow \mathrm{Aut}(\mathbb{A}) \tag{3.12}$$

giving the canonical actions of $\mathcal{G}$ on F and $\mathbb{A}$, respectively. Besides, for any $m \geq 1$, we obtain two homomorphisms

$$\tau^0_m : \mathcal{G}_m \longrightarrow Z^1\big(F, \overline{\mathsf{A}}_m\big) \quad \text{and} \quad \tau^1_m : \mathcal{G}_m \longrightarrow \mathrm{Hom}\big(\mathbb{A}, \overline{\mathsf{A}}_{m+1}\big), \tag{3.13}$$

which maps any $g \in \mathcal{G}_m$ to

$$\big([x]_0 \longmapsto [g(x)x^{-1}]_m\big) \quad \text{and} \quad \big([a]_1 \mapsto [g(a)a^{-1}]_{m+1}\big),$$

respectively. Note that, for all $m \geq 0$, we have

$$\ker \tau_m^0 = \mathcal{G}_{m+1}^0 \quad \text{and} \quad \ker \tau_m^1 = \mathcal{G}_{m+1}^1 = \mathcal{G}_{m+1}. \tag{3.14}$$

In the sequel, the homomorphisms τ_i^0 and τ_i^1 (for $i \geq 0$) are called the *Johnson homomorphisms* for the automorphism group of the free pair (π, A).

Remark 3.3. The two sequences of homomorphisms, $(\tau_i^0)_{i\geq 0}$ and $(\tau_i^1)_{i\geq 0}$, are defined on the successive terms of the filtration $\mathcal{G}_*$, rather than on $\mathcal{G}_*^0$. Nonetheless,

(1) if restricted to $\mathcal{G}_{m+1}^0 \subset \mathcal{G}_m$, the homomorphism τ_m^1 takes values in $\mathrm{Aut}_{\mathbb{Z}[F]}(\mathbb{A})$ $\big($resp. in $\mathrm{Hom}_{\mathbb{Z}[F]}\big(\mathbb{A}, \overline{\mathsf{A}}_{m+1}\big)\big)$ for $m = 0$ (resp. for $m \geq 1$),

(2) and the homomorphism τ_m^0 extends on $\mathcal{G}_m^0 \supset \mathcal{G}_m$ to a homomorphism (resp. to a 1-cocycle) for $m \geq 2$ (resp. for $m = 1$):

$$\begin{tikzcd}
\mathcal{G}_m^0 \arrow[r, dashed, "\tilde{\tau}_m^0"] & Z^1\big(\pi, \overline{\mathsf{A}}_m\big) \\
\mathcal{G}_m \arrow[u, hook] \arrow[r, "\tau_m^0"] & Z^1\big(F, \overline{\mathsf{A}}_m\big). \arrow[u]
\end{tikzcd}$$

See [HM18, Proposition 10.5] and [HM18, Proposition 10.6].

Remark 3.4. When $\mathsf{A} = \pi$, we have $\mathcal{G}_{m+1}^0 = \mathcal{G}_m$ and τ_m^0 is trivial for all $m \geq 0$. Then, we get the usual theory of Johnson homomorphisms for the automorphism group $\mathrm{Aut}(\pi)$ of the free group π. See [Sa16] for a survey.

For the reader's convenience, we now write down the various properties of the Johnson homomorphisms $(\tau_i^0)_{i\geq 0}$ and $(\tau_i^1)_{i\geq 0}$ that are directly inherited from the properties of the Johnson morphism $\overline{\tau}_\bullet$:

- For any $g \in \mathcal{G}_0$, the two components $\tau_0^0(g), \tau_0^1(g)$ of $\overline{\tau}_0(g)$ are related by

$$\tau_0^1(g)({}^x a) = {}^{\tau_0^0(g)(x)}\big(\tau_0^1(g)(a)\big) \quad \text{for all } x \in F,\ a \in \mathbb{A} \tag{3.15}$$

  and, for any $g \in \mathcal{G}_m$ and $m \geq 1$, the two components $\tau_m^0(g), \tau_m^1(g)$ of $\overline{\tau}_m(g)$ are related by

$$\tau_m^1(g)({}^x a) = {}^x\big(\tau_m^1(g)(a)\big) + \big[\tau_m^0(g)(x), {}^x a\big] \quad \text{for all } x \in F,\ a \in \mathbb{A}. \tag{3.16}$$

  (Identity (3.15) corresponds to the equivariance of the automorphism $\overline{\tau}_0(g)$ of the extended graded Lie algebra $\overline{\mathsf{A}}_\bullet$, and identity (3.16) is the defect of F-equivariance of the degree m derivation $\overline{\tau}_m(g)$ of the extended graded Lie algebra $\overline{\mathsf{A}}_\bullet$.)
- For any $g \in \mathcal{G}_m$ $(m \geq 1)$ and $h \in \mathcal{G}_n$ $(n \geq 1)$, we can compute $t_0 := \tau_{m+n}^0([g,h])$ as well as $t_1 := \tau_{m+n}^1([g,h])$ from $d_i := \tau_m^i(g), i \in \{0,1\}$ and $e_j := \tau_n^j(h), j \in \{0,1\}$ by

$$t_0(x) \;=\; d_n(e_0(x)) - e_m(d_0(x)) - [d_0(x), e_0(x)] \quad \text{for all } x \in F, \tag{3.17}$$

$$t_1(a) \;=\; d_{n+1}(e_1(a)) - e_{m+1}(d_1(a)) \quad \text{for all } a \in \mathbb{A}, \tag{3.18}$$

  where $d_+ = (d_i)_{i\geq 1}$ and $e_+ = (e_i)_{i\geq 1}$ denote the derivations of $\mathrm{Lie}(\mathbb{A}) = \overline{\mathsf{A}}_+$ that extend d_1 and e_1, respectively. (These identities correspond to the fact that $\overline{\tau}_+$ is a homomorphism of graded Lie algebras.)

- For all $g \in \mathcal{G}$ and $h \in \mathcal{G}_m$ $(m \geq 1)$, we have

$$\tau^0_m({}^g h) \quad = \quad \mathrm{Lie}_m(\tau^1_0(g)) \circ \tau^0_m(h) \circ \tau^0_0(g)^{-1}, \tag{3.19}$$

$$\tau^1_m({}^g h) \quad = \quad \mathrm{Lie}_{m+1}(\tau^1_0(g)) \circ \tau^1_m(h) \circ \tau^1_0(g)^{-1}, \tag{3.20}$$

where $\mathrm{Lie}(\tau^1_0(g))$ is the automorphism of $\mathrm{Lie}(\mathbb{A}) = \overline{\mathsf{A}}_+$ induced by $\tau^1_0(g) \in \mathrm{Aut}(\mathbb{A})$. (These identities correspond to the equivariance of $\overline{\tau}_+$ over $\overline{\tau}_0$.)

3.3. **Formality of free pairs.** We shall prove that the extended N-series A_* is formal in the sense of §2.2. For this, we work over $\mathbb{Q}$.

Since $\overline{\mathsf{A}}^{\mathbb{Q}}_+$ is the free Lie $\mathbb{Q}$-algebra on $\mathbb{A}^{\mathbb{Q}} := \mathbb{A} \otimes \mathbb{Q}$, the universal enveloping algebra of the extended graded Lie algebra $\overline{\mathsf{A}}^{\mathbb{Q}}_\bullet$ is

$$U\big(\overline{\mathsf{A}}^{\mathbb{Q}}_\bullet\big) = U\big(\overline{\mathsf{A}}^{\mathbb{Q}}_+\big) \otimes_{\mathbb{Q}} \mathbb{Q}[F] = T(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F],$$

where $T(\mathbb{A}^{\mathbb{Q}})$ is the tensor algebra of $\mathbb{A}^{\mathbb{Q}}$. (The multiplication in $U\big(\overline{\mathsf{A}}^{\mathbb{Q}}_\bullet\big)$ is given by (2.4)). So, for degree-completions, we have

$$\widehat{U}(\overline{\mathsf{A}}^{\mathbb{Q}}_\bullet) = T(\mathbb{A}^{\mathbb{Q}}) \,\hat{\otimes}_{\mathbb{Q}}\, \mathbb{Q}[F] := \prod_{m \geq 0} \big((\mathbb{A}^{\mathbb{Q}})^{\otimes m} \otimes_{\mathbb{Q}} \mathbb{Q}[F]\big),$$

which strictly contains $\widehat{T}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F] = \big(\prod_{m\geq 0} (\mathbb{A}^{\mathbb{Q}})^{\otimes m}\big) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$.

Definition 3.5. An *expansion* of the free pair (π, A) is a monoid homomorphism

$$\theta : \pi \longrightarrow \widehat{T}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$$

for which there is a map ℓ^θ from π to the degree-completion of $\mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ such that

$$\theta(x) \quad = \quad \exp\big(\ell^\theta(x)\big) \otimes \varpi(x) \quad \text{for all } x \in \pi, \tag{3.21}$$

$$\ell^\theta(a) \quad = \quad [a]_1 + (\deg \geq 2) \quad \text{for any } a \in \mathsf{A}. \tag{3.22}$$

From [HM18, Lemma 11.1], which identifies the group-like part of $\widehat{U}(\overline{\mathsf{A}}^{\mathbb{Q}}_\bullet)$, it follows that an expansion of the free pair (π, A) in the sense of Definition 3.5 is the same as an expansion of the extended N-series A_* in the sense of §2.2.

Lemma 3.6. *There exists an expansion θ of (π, A). In particular, the extended N-series A_* is formal.*

Proof. Let $\{\alpha_i\}_{i\in I} \sqcup \{\beta_j\}_{j \in J}$ be a basis of π of type (3.1). We set $a_i = [\alpha_i]_1 \in \mathbb{A}$ for every $i \in I$, and $x_j = [\beta_j]_0 \in F$ for every $j \in J$. Let $\theta : \pi \to \widehat{T}(\mathbb{A}^{\mathbb{Q}}) \otimes \mathbb{Q}[F]$ be the monoid homomorphism such that

$$\theta(\alpha_i) = \exp(a_i) \otimes 1 = \sum_{k \geq 0} \frac{a_i^k}{k!} \otimes 1 \quad \text{and} \quad \theta(\beta_j) = 1 \otimes x_j.$$

For any $\ell, \ell' \in \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ and $f, f' \in F$, we have

$$\begin{aligned} \big(\exp(\ell) \otimes f\big) \cdot \big(\exp(\ell') \otimes f'\big) \quad &= \quad \big(\exp(\ell) \exp({}^f\ell')\big) \otimes (ff') \\ &= \quad \exp\Big(\ell + {}^f\ell' + \frac{1}{2}[\ell, {}^f\ell'] + \cdots\Big) \otimes (ff'). \end{aligned}$$

Since π is generated by $\alpha \sqcup \beta$, the BCH formula implies that there is a unique map ℓ^θ satisfying (3.21). Furthermore, we have

$$\ell^\theta(xx') = \ell^\theta(x) + {}^{\varpi(x)}\big(\ell^\theta(x')\big) + \frac{1}{2}\big[\ell^\theta(x), {}^{\varpi(x)}\big(\ell^\theta(x')\big)\big] + \cdots \tag{3.23}$$

for all $x, x' \in \pi$, where the terms not shown are Lie commutators of $\ell^\theta(x)$ and ${}^{\varpi(x)}\big(\ell^\theta(x')\big)$ of higher length.

Let $\widetilde{\mathsf{A}}$ be the subset of A consisting of the elements a satisfying (3.22). Clearly $\widetilde{\mathsf{A}}$ contains α. By (3.23), $\widetilde{\mathsf{A}}$ is stable under multiplication, hence under conjugation by elements of α. Besides, $\widetilde{\mathsf{A}}$ is stable under conjugation by elements of β since we have, for any $a \in \widetilde{\mathsf{A}}$ and $j \in J$,

$$\begin{aligned}
\theta(\beta_j a \beta_j^{-1}) &= (1 \otimes \varpi(\beta_j)) \cdot \big(\exp(\ell^\theta(a)) \otimes 1\big) \cdot (1 \otimes \varpi(\beta_j)^{-1}) \\
&= \exp\big({}^{\varpi(\beta_j)}(\ell^\theta(a))\big) \otimes 1 \\
&= \exp\big({}^{\varpi(\beta_j)}([a]_1) + (\deg \geq 2)\big) \otimes 1
\end{aligned}$$

so that $\beta_j a \beta_j^{-1}$ belongs to $\widetilde{\mathsf{A}}$. We conclude that $\widetilde{\mathsf{A}} = \mathsf{A}$. □

Recall that $\mathcal{G}_1$ is the subgroup of $\mathcal{G}$ acting trivially on the abelianization $\mathbb{A}$ of A. The complete Lie algebra $\widehat{D}_+\big(\overline{\mathsf{A}}_\bullet^{\mathbb{Q}}\big)$ is viewed as a group with multiplication given by the BCH formula.

Theorem 3.7. *Let θ be an expansion of the free pair (π, A). There is a group homomorphism*

$$\varrho^\theta : \mathcal{G}_1 \longrightarrow \widehat{D}_+\big(\overline{\mathsf{A}}_\bullet^{\mathbb{Q}}\big) \tag{3.24}$$

whose restriction to $\mathcal{G}_m$ $(m \geq 1)$ starts in degree m with (τ_m^0, τ_m^1). Furthermore, ϱ^θ is injective.

Proof. The first statement is a specialization of (2.6) to the extended N-series A_* for the free pair (π, A). Indeed, since $\overline{\mathsf{A}}_+ = \mathrm{Lie}(\mathbb{A})$ is a torsion-free abelian group, there is no loss of information in considering the rational version $\overline{\tau}_+^{\mathbb{Q}}$ instead of $\overline{\tau}_+$ [HM18, Remark 12.8]. Furthermore, we use here the "truncation" isomorphism $\mathrm{Der}_+(\overline{\mathsf{A}}_\bullet^{\mathbb{Q}}) \simeq D_+(\overline{\mathsf{A}}_\bullet^{\mathbb{Q}})$.

The second statement is a direct consequence of (3.4). □

4. First terms of the Johnson filtration for a free pair

Let $p, q \geq 0$ be integers with either $p \geq 2$ or $p, q \geq 1$. We assume that π is a free group with basis $\alpha \sqcup \beta = \{\alpha_1, \ldots, \alpha_p\} \sqcup \{\beta_1, \ldots, \beta_q\}$ and that

$$\mathsf{A} := \langle\!\langle \alpha_1, \ldots, \alpha_p \rangle\!\rangle.$$

Set $F := \pi/\mathsf{A}$ and let $\varpi : \pi \to F$ be the canonical projection. Then F is a free group with basis $(x_1, \ldots, x_q)$, where $x_j := \varpi(\beta_j)$ for each $j \in \{1, \ldots, q\}$. Hence (π, A) is a free pair. In this section, we compute the first few terms of the Johnson filtration for $\mathrm{Aut}(\pi, \mathsf{A})$.

4.1. **Magnus representations for a free pair.** Let $\mathbb{Z}[\pi]$ be the group algebra of π. Let $\varepsilon : \mathbb{Z}[\pi] \to \mathbb{Z}$ be the augmentation, and $\overline{\,\cdot\,} : \mathbb{Z}[\pi] \to \mathbb{Z}[\pi]$ the linear map defined by $\overline{u} = u^{-1}$ for all $u \in \pi$. Consider the (left) Fox derivatives with respect to the basis (α, β) of π, which are the linear maps

$$\frac{\partial}{\partial \alpha_i} : \mathbb{Z}[\pi] \longrightarrow \mathbb{Z}[\pi] \quad (i = 1, \ldots, p) \quad \text{and} \quad \frac{\partial}{\partial \beta_j} : \mathbb{Z}[\pi] \longrightarrow \mathbb{Z}[\pi] \quad (j = 1, \ldots, q)$$

defined by

$$w-\varepsilon(w)=\sum_{i=1}^{p}\frac{\partial w}{\partial \alpha_i}(\alpha_i-1)+\sum_{j=1}^{q}\frac{\partial w}{\partial \beta_j}(\beta_j-1)\quad \text{for all } w\in \mathbb{Z}[\pi]. \tag{4.1}$$

We associate to every $g \in \mathrm{Aut}(\pi)$ its *free Jacobian matrix* with respect to the basis $\alpha \sqcup \beta$ of π:

$$J(g) := \begin{pmatrix} \overline{\frac{\partial g(\alpha_1)}{\partial \alpha_1}} & \cdots & \overline{\frac{\partial g(\alpha_p)}{\partial \alpha_1}} & \overline{\frac{\partial g(\beta_1)}{\partial \alpha_1}} & \cdots & \overline{\frac{\partial g(\beta_q)}{\partial \alpha_1}} \\ \vdots & & \vdots & \vdots & & \vdots \\ \overline{\frac{\partial g(\alpha_1)}{\partial \alpha_p}} & \cdots & \overline{\frac{\partial g(\alpha_p)}{\partial \alpha_p}} & \overline{\frac{\partial g(\beta_1)}{\partial \alpha_p}} & \cdots & \overline{\frac{\partial g(\beta_q)}{\partial \alpha_p}} \\ \overline{\frac{\partial g(\alpha_1)}{\partial \beta_1}} & \cdots & \overline{\frac{\partial g(\alpha_p)}{\partial \beta_1}} & \overline{\frac{\partial g(\beta_1)}{\partial \beta_1}} & \cdots & \overline{\frac{\partial g(\beta_q)}{\partial \beta_1}} \\ \vdots & & \vdots & \vdots & & \vdots \\ \overline{\frac{\partial g(\alpha_1)}{\partial \beta_q}} & \cdots & \overline{\frac{\partial g(\alpha_p)}{\partial \beta_q}} & \overline{\frac{\partial g(\beta_1)}{\partial \beta_q}} & \cdots & \overline{\frac{\partial g(\beta_q)}{\partial \beta_q}} \end{pmatrix} \in \mathrm{GL}(p+q;\mathbb{Z}[\pi]).$$

In the sequel, we use the notations of §3.1. In particular, set $\mathcal{G} = \mathrm{Aut}(\pi, \mathsf{A})$. Let $J^F : \mathcal{G} \to \mathrm{GL}(p+q;\mathbb{Z}[F])$ be the map obtained by restricting $J : \mathrm{Aut}(\pi) \to \mathrm{GL}(p+q;\mathbb{Z}[\pi])$ to $\mathcal{G}$ and by applying ϖ to each matrix entry. The next proposition identifies the four blocks (namely $p\times p$, $p\times q$, $q\times p$ and $q \times q$) of the corresponding matrices.

Proposition 4.1. (1) *The lower-left block of J^F is trivial.*

(2) *The lower-right block of J^F defines a crossed homomorphism*

$$\mathrm{Mag}_0^0 : \mathcal{G} \longrightarrow \mathrm{GL}(q;\mathbb{Z}[F]), \quad g \longmapsto \left(\varpi\Big(\overline{\frac{\partial g(\beta_j)}{\partial \beta_i}}\Big)\right)_{i,j}$$

which is equivalent to $\tau_0^0 : \mathcal{G} \to \mathrm{Aut}(F)$ (in the sense that Mag_0^0 factors through an injective crossed homomorphism $\mathrm{Aut}(F) \to \mathrm{GL}(q;\mathbb{Z}[F])$).

(3) *The upper-left block of J^F defines a crossed homomorphism*

$$\mathrm{Mag}_0^1 : \mathcal{G} \longrightarrow \mathrm{GL}(p;\mathbb{Z}[F]), \quad g \longmapsto \left(\varpi\Big(\overline{\frac{\partial g(\alpha_j)}{\partial \alpha_i}}\Big)\right)_{i,j}$$

which, with the knowledge of Mag_0^0, is equivalent to $\tau_0^1 : \mathcal{G} \to \mathrm{Aut}(\mathbb{A})$.

(4) *The upper-right block of J^F restricts to a homomorphism*

$$\mathrm{Mag}_1^0 : \mathcal{G}_1 \longrightarrow \mathrm{Mat}(p\times q;\mathbb{Z}[F]), \quad g \longmapsto \left(\varpi\Big(\overline{\frac{\partial g(\beta_j)}{\partial \alpha_i}}\Big)\right)_{i,j}$$

which is equivalent to $\tau_1^0 : \mathcal{G}_1 \to Z^1(F,\mathbb{A})$ (in the sense that Mag_1^0 factors through an injective homomorphism $Z^1(F,\mathbb{A}) \to \mathrm{Mat}(p\times q;\mathbb{Z}[F])$).

The next lemma, which follows from elementary properties of Fox derivatives, is needed for the proof of Proposition 4.1.

Lemma 4.2. *The map $\kappa : \mathbb{A} \to \mathbb{Z}[F]^p$ defined by*

$$\kappa([a]) = \Big(\varpi\big(\frac{\partial a}{\partial \alpha_1}\big), \ldots, \varpi\big(\frac{\partial a}{\partial \alpha_p}\big)\Big) \tag{4.2}$$

is an isomorphism of $\mathbb{Z}[F]$-modules, where $\mathbb{Z}[F]$ acts on $\mathbb{Z}[F]^p$ by left multiplication.

Proof. For any $a_1, a_2 \in \mathsf{A}$, and for all $i \in \{1, \dots, g\}$, we have

$$\varpi\Big(\frac{\partial(a_1 a_2)}{\partial \alpha_i}\Big) = \varpi\Big(\frac{\partial a_1}{\partial \alpha_i}\Big) + \varpi\Big(a_1 \frac{\partial a_2}{\partial \alpha_i}\Big) = \varpi\Big(\frac{\partial a_1}{\partial \alpha_i}\Big) + \varpi\Big(\frac{\partial a_2}{\partial \alpha_i}\Big).$$

This shows that the right side of (4.2) defines a homomorphism $\mathsf{A} \to \mathbb{Z}[F]^p$ and, since the group $\mathbb{Z}[F]^p$ is abelian, κ is a well-defined homomorphism.

Let $i \in \{1, \dots, p\}$, $a \in \mathsf{A}$ and $w \in \pi$. We have

$$\varpi\Big(\frac{\partial(waw^{-1})}{\partial \alpha_i}\Big) \;=\; \varpi\Big(\frac{\partial w}{\partial \alpha_i}\Big) + \varpi\Big(w\frac{\partial a}{\partial \alpha_i}\Big) + \varpi\Big(wa\frac{\partial w^{-1}}{\partial \alpha_i}\Big) \;=\; \varpi(w)\varpi\Big(\frac{\partial a}{\partial \alpha_i}\Big),$$

which shows that the map κ is $\mathbb{Z}[F]$-linear.

By Lemma 3.2, the $\mathbb{Z}[F]$-module $\mathbb{A}$ is free on the classes of $\alpha_1, \dots, \alpha_p$. This basis of $\mathbb{A}$ is sent by κ to the canonical basis of $\mathbb{Z}[F]^p$. Hence κ is an isomorphism. $\square$

Proof of Proposition 4.1. It is well known that J is a crossed homomorphism, i.e.,

$$J(gg') = J(g) \cdot g\big(J(g')\big) \quad \text{for all } g, g' \in \mathrm{Aut}(\pi),$$

see e.g. [Bir74, §3]. Hence, we get

$$J^F(gg') = J^F(g) \cdot g^F\big(J^F(g')\big) \quad \text{for all } g, g' \in \mathcal{G}, \tag{4.3}$$

where we set $g^F := \tau_0^0(g) \in \mathrm{Aut}(F)$ for all $g \in \mathcal{G}$.

Let $g \in \mathcal{G}$. Then $g(\alpha_i) \in \mathsf{A}$ for all $i \in \{1, \dots, p\}$. Thus, statement (1) follows since, for any $a \in \mathsf{A}$ and for all $j \in \{1, \dots, q\}$, we have

$$\varpi\Big(\frac{\partial a}{\partial \beta_j}\Big) = 0. \tag{4.4}$$

Note that, for any $a', a'' \in \mathsf{A}$, we have

$$\varpi\Big(\frac{\partial a' a''}{\partial \beta_j}\Big) = \varpi\Big(\frac{\partial a'}{\partial \beta_j} + a'\frac{\partial a''}{\partial \beta_j}\Big) = \varpi\Big(\frac{\partial a'}{\partial \beta_j}\Big) + \varpi\Big(\frac{\partial a''}{\partial \beta_j}\Big).$$

Thus, it is enough to prove (4.4) for $a = w\alpha_k w^{-1}$, where $k \in \{1, \dots, p\}$ and $w \in \pi$:

$$\begin{aligned} \varpi\Big(\frac{\partial w\alpha_k w^{-1}}{\partial \beta_j}\Big) \;&=\; \varpi\Big(\frac{\partial w}{\partial \beta_j}\Big) + \varpi(w)\,\varpi\Big(\frac{\partial \alpha_k w^{-1}}{\partial \beta_j}\Big) \\ &=\; \varpi\Big(\frac{\partial w}{\partial \beta_j}\Big) + \varpi(w)\,\varpi\Big(\frac{\partial w^{-1}}{\partial \beta_j}\Big) \;=\; \varpi\Big(\frac{\partial ww^{-1}}{\partial \beta_j}\Big) \;=\; 0. \end{aligned}$$

We deduce from statement (1) and from (4.3) that the two diagonal blocks of J^F define crossed homomorphisms with values in general linear groups.

Let $g \in \mathcal{G}$. Then $g^F = \tau_0^0(g) \in \mathrm{Aut}(F)$ is determined by its free Jacobian matrix with respect to the basis $\{x_1, \dots, x_q\}$. Thus, statement (2) will follow since the latter is equal to the lower-right block of J^F. Indeed, for all $r \in \{1, \dots, q\}$, we have

$$g(\beta_r) - 1 = \sum_i \frac{\partial g(\beta_r)}{\partial \alpha_i}(\alpha_i - 1) + \sum_j \frac{\partial g(\beta_r)}{\partial \beta_j}(\beta_j - 1).$$

Therefore, by applying ϖ, we get

$$g^F(x_r) - 1 = \sum_j \varpi\Big(\frac{\partial g(\beta_r)}{\partial \beta_j}\Big)(x_j - 1)$$

which implies that

$$\varpi\Big(\frac{\partial g(\beta_r)}{\partial \beta_j}\Big) = \frac{\partial g^F(x_r)}{\partial x_j} \text{ for all } j \in \{1,\dots,q\}.$$

Let $g \in \mathcal{G}$. Since the pair $(\tau_0^0(g), \tau_0^1(g))$ satisfies (3.15), the automorphism $\tau_0^1(g)$ is determined by its values on the basis $\{[\alpha_1],\dots,[\alpha_p]\}$ and by $\tau_0^0(g)$. The converse is also true since $\mathbb{A}$ is torsion-free as a $\mathbb{Z}[F]$-module. Besides, Lemma 4.2 implies that the upper-left block of $J^F(g)$ contains as much information as $[g(\alpha_1)],\dots,[g(\alpha_p)] \in \mathbb{A}$. Thus we have proved statement (3).

We conclude with the proof of statement (4). First observe that the diagonal blocks of J^F on $\mathcal{G}_1$ are identity blocks since $\mathcal{G}_1 = \ker \tau_0^1$. Thus, the upper-right block of $J^F : \mathcal{G}_1 \to \mathrm{GL}(p+q;\mathbb{Z}[F])$ is a homomorphism. Let $g \in \mathcal{G}_1$. The 1-cocycle $\tau_1^0(g)$ is determined by its values on the basis $\{x_1,\dots,x_q\}$ of F. For each $j \in \{1,\dots,q\}$, the value of $\tau_1^0(g)$ on x_j is $[g(\beta_j)\beta_j^{-1}] \in \mathbb{A}$ and, for all $i \in \{1,\dots,p\}$,

$$\varpi\Big(\frac{\partial(g(\beta_j)\beta_j^{-1})}{\partial \alpha_i}\Big) = \varpi\Big(\frac{\partial g(\beta_j)}{\partial \alpha_i}\Big).$$

Hence, according to Lemma 4.2, the value of $\tau_1^0(g)$ on x_j is encoded by (the conjugate of) the j-th column of the upper-right block of $J^F(g)$. □

4.2. **The quotient $\mathcal{G}/\mathcal{G}_1^0$.** Let us consider the first four terms of the filtration (3.3):

$$\mathcal{G} = \mathcal{G}_0 \geq \mathcal{G}_1^0 \geq \mathcal{G}_1 \geq \mathcal{G}_2^0 \tag{4.5}$$

The homomorphism $\tau_0^0 : \mathcal{G} \to \mathrm{Aut}(F)$ is split surjective since any automorphism of $\langle \beta_1,\dots,\beta_q\rangle \simeq F$ extends to an automorphism of (π, A) that fixes each of $\alpha_1,\dots,\alpha_p$. Hence τ_0^0 induces an isomorphism $\mathcal{G}/\mathcal{G}_1^0 \simeq \mathrm{Aut}(F)$. Also, we can identify $\mathcal{G}/\mathcal{G}_1^0$ with a subset of $\mathrm{GL}(q;\mathbb{Z}[F])$ via the crossed homomorphism Mag_0^0.

In the rest of this section, we study the next two successive quotients in (4.5).

4.3. **The quotient $\mathcal{G}_1^0/\mathcal{G}_1$.** Let us now consider the quotient $\mathcal{G}_1^0/\mathcal{G}_1$. It embeds into $\mathrm{Aut}_{\mathbb{Z}[F]}(\mathbb{A})$ via τ_0^1 (see Remark 3.3). Equivalently, $\mathcal{G}_1^0/\mathcal{G}_1$ embeds into $\mathrm{GL}(p;\mathbb{Z}[F])$ via Mag_0^1. Consider the homomorphism

$$r := \mathrm{Mag}_0^1|_{\mathcal{G}_1^0} : \mathcal{G}_1^0 \to \mathrm{GL}(p;\mathbb{Z}[F]).$$

We have $\ker(r) = \ker(\tau_0^1) \cap \mathcal{G}_1^0 = \mathcal{G}_1^1 \cap \mathcal{G}_1^0 = \mathcal{G}_1$. Thus, we have an exact sequence

$$1 \longrightarrow \mathcal{G}_1 \longrightarrow \mathcal{G}_1^0 \stackrel{r}{\longrightarrow} \mathrm{GL}(p;\mathbb{Z}[F]). \tag{4.6}$$

Now, it remains to identify the image of r (or, equivalently, the image of τ_0^1 in $\mathrm{Aut}_{\mathbb{Z}[F]}(\mathbb{A}) \simeq \mathrm{GL}(p;\mathbb{Z}[F])$). We give below a partial answer.

Let R be a (associative, unital) ring, and let $U(R)$ be its group of units. The *general elementary subgroup* $\mathrm{GE}(p;R)$ of $\mathrm{GL}(p;R)$ is generated by invertible diagonal matrices and elementary matrices, i.e., it is generated by

- $d_i(u) := I_p + (u-1)E_{ii}$ for $i \in \{1,\dots,p\}$ and $u \in U(R)$,
- $e_{ij}(w) := I_p + wE_{ij}$ for $i,j \in \{1,\dots,p\}$, $i \neq j$, and $w \in R$.

Following Cohn [Co66], a ring R is said to be *generalized euclidean* if $\mathrm{GE}(p;R) = \mathrm{GL}(p;R)$ for every $p \geq 2$. Of course, generalized euclidean rings include ordinary euclidean rings (as a consequence of the Gauss algorithm). We are interested here in the ring $R := \mathbb{Z}[F]$ for a free group F of rank q, but it does not seem to be known whether it is generalized euclidean or not (even in the case $q = 1$ [Guy16]).

Remark 4.3. The group algebra $\mathbb{Q}[F]$ with coefficients in $\mathbb{Q}$ is generalized euclidean [Co66, Theorem 3.4], but free associative rings (including the 1-variable polynomial ring $\mathbb{Z}[X]$) are not [Co66, end of §8].

The following gives a partial information on $r(\mathcal{G}_1^0) \simeq \mathcal{G}_1^0/\mathcal{G}_1$.

Proposition 4.4. *We have* $\mathrm{GE}(p;\mathbb{Z}[F]) \leq r(\mathcal{G}_1^0) \leq \mathrm{GL}(p;\mathbb{Z}[F])$.

In the rest of this section, we use the following notations for endomorphisms of the free group $\pi = \langle \alpha_1, \dots, \alpha_p, \beta_1, \dots, \beta_q \rangle$. For distinct generators $u_1, \dots, u_r \in \{\alpha_i\}_i \sqcup \{\beta_j\}_j$ and elements $v_1, \dots, v_r \in \pi$, let $(u_1 \mapsto v_1, \dots, u_r \mapsto v_r)$ denote the endomorphism of π sending u_i to y_i for $i = 1, \dots, r$ and each of the other generators to itself.

Proof of Proposition 4.4. Recall that $U(\mathbb{Z}[F]) = \pm F$ by a classical result of Higman [Hig40]. Hence $\mathrm{GE}(p;\mathbb{Z}[F])$ is generated by the matrices $d_i(\epsilon x)$ with $\epsilon = \pm 1$ and $x \in F$ and the matrices $e_{ij}(x)$ with $x \in F$. All these matrices belong to the image of r:

- we have $r\big(\tilde{d}_i(\epsilon x)\big) = d_i(\epsilon x)$, where $\tilde{d}_i(\epsilon x) := \big(\alpha_i \mapsto {}^{x^{-1}}\alpha_i^{\epsilon}\big) \in \mathcal{G}_1^0$ (here and below, we are identifying $x \in F$ with a lift in $B \leq \pi$);
- we have $r(\tilde{e}_{ij}(x)) = e_{ij}(x)$, where $\tilde{e}_{ij}(x) := \big(\alpha_j \mapsto ({}^{x^{-1}}\alpha_i)\, \alpha_j\big) \in \mathcal{G}_1^0$.

□

Remark 4.5. For any group G, the general elementary groups $\mathrm{GE}(p;\mathbb{Z}[G])$ are used in the definition of the *Whitehead group*:

$$\mathrm{Wh}(G) = \varinjlim_p \mathrm{GL}(p;\mathbb{Z}[G]) / \varinjlim_p \mathrm{GE}(p;\mathbb{Z}[G]).$$

According to [Sta65], the Whitehead group $\mathrm{Wh}(F)$ of the free group $F = F_q$ of rank q is trivial. Hence the surjectivity of $r = r_{p,q}$ holds stably in p, i.e., for any fixed $q \geq 0$, the inductive limit

$$\varinjlim_p r_{p,q} : \varinjlim_p (\mathcal{G}_{p,q})_1^0 \to \varinjlim_p \mathrm{GL}(p;\mathbb{Z}[F_q]),$$

is surjective.

4.4. The quotient $\mathcal{G}_1/\mathcal{G}_2^0$.

We now identify $\mathcal{G}_1/\mathcal{G}_2^0$.

Proposition 4.6. *We have the short exact sequence*

$$1 \longrightarrow \mathcal{G}_2^0 \longrightarrow \mathcal{G}_1 \xrightarrow{\tau_1^0} Z^1(F,\mathbb{A}) \longrightarrow 1 \tag{4.7}$$

or, equivalently, we have the short exact sequence

$$1 \longrightarrow \mathcal{G}_2^0 \longrightarrow \mathcal{G}_1 \xrightarrow{\mathrm{Mag}_1^0} \mathrm{Mat}(p \times q;\mathbb{Z}[F]) \longrightarrow 1. \tag{4.8}$$

Thus we have $\mathcal{G}_1/\mathcal{G}_2^0 \simeq Z^1(F,\mathbb{A}) \simeq \mathrm{Mat}(p \times q;\mathbb{Z}[F])$.

Proof. The equivalence of (4.7) and (4.8) follows directly from the sequence of isomorphisms

$$Z^1(F,\mathbb{A}) \simeq \mathbb{A}^q \simeq (\mathbb{Z}[F]^p)^q = \mathrm{Mat}(p \times q;\mathbb{Z}[F]) \tag{4.9}$$

through which τ_1^0 corresponds to Mag_1^0. (See the proof of Proposition 4.1.(4).) Hence it suffices to prove that τ_1^0 is surjective.

For $i \in \{1,\dots,q\}$, $s \in \{1,\dots,p\}$, $b \in \langle \beta_1,\dots,\beta_q\rangle$, set

$$\varphi_{i,s,b} := (\alpha_s \mapsto {}^b\alpha_s) \circ (\beta_i \mapsto \alpha_s\beta_i) \circ (\alpha_s \mapsto {}^b\alpha_s)^{-1}.$$

Since $(\beta_i \mapsto \alpha_s\beta_i) \in \mathcal{G}_1$ and $(\alpha_s \mapsto {}^b\alpha_s) \in \mathcal{G}$, we have $\varphi_{i,s,b} \in \mathcal{G}_1$. Observe that $\varphi_{i,s,b}(\beta_i) = {}^b\alpha_s\beta_i$, and $\varphi_{i,s,b}(\beta_j) = \beta_j$ for $j \neq i$. Hence, we have

$$\tau_1^0(\varphi_{i,s,b})(x_j) = \left[({}^b\alpha_s)^{\delta_{j,i}}\right] \in \mathbb{A}.$$

Since the $\tau_1^0(\varphi_{i,s,b})$ form a basis of the free abelian group $Z^1(F,\mathbb{A})$, it follows that τ_1^0 is surjective. □

5. The Johnson filtration for the handlebody group

We now review some basic facts about the handlebody group, and we start the study of the Johnson filtration in this situation.

5.1. **The handlebody group $\mathcal{H}$.** Let V be a handlebody of genus g. Let D be a disk in ∂V, and set $\Sigma := \partial V \setminus \mathrm{int}(D)$. Let $\mathcal{H}$ be the mapping class group of V rel D, which is called the *handlebody group*. Let $\mathcal{M}$ be the mapping class group of Σ rel $\partial\Sigma$. By restricting self-homeomorphisms of V to Σ, we obtain an injective homomorphism $\mathcal{H} \to \mathcal{M}$ (see e.g. [Hen18, §3]). Thus we regard $\mathcal{H}$ as a subgroup of $\mathcal{M}$.

Choose a base point $\star \in \partial D$, and define the *twist group*

$$\mathcal{T} := \ker\big(\mathcal{H} \longrightarrow \mathrm{Aut}(\pi_1(V,\star))\big)$$

as the subgroup of $\mathcal{H}$ acting trivially on the fundamental group of V. A *disk-twist* is the isotopy class of self-homeomorphisms of V defined by twisting V along a properly embedded disk U in V (see e.g. [Hen18, §5]). The corresponding element of $\mathcal{H} \subset \mathcal{M}$ is the Dehn twist $T_{\partial U}$ along the simple closed curve ∂U, which is a *meridian* of V. Thus, disk-twists are also called "meridional Dehn twists" in the literature.

In the following, we derive two results on the handlebody group $\mathcal{H}$ of V rel D from results of Luft [Lu78] and Griffiths [Gri64] on the handlebody group of V rel $\star$.

Theorem 5.1 (Luft)**.** *The subgroup $\mathcal{T}$ of $\mathcal{H}$ is generated by disk-twists. In other words, the subgroup $\mathcal{T}$ of $\mathcal{M}$ is generated by Dehn twists along meridians (i.e. simple closed curves of Σ null-homotopic in V).*

Proof. This is derived from Luft's theorem [Lu78]. Let $\mathcal{T}_\circ$ be the subgroup of $\mathcal{H}$ generated by disk-twists. Since any disk-twist acts trivially on $\pi_1(V,\star)$, we have $\mathcal{T}_\circ \subset \mathcal{T}$. It remains to prove the converse inclusion.

Let $\hat{\mathcal{M}}$ and $\hat{\mathcal{H}}$ be the mapping class groups of ∂V and V, respectively, rel $\star$. Let $\hat{\mathcal{T}}$ denote the twist group for V rel $\star$, which is defined as the kernel of the canonical map $\hat{\mathcal{H}} \to \mathrm{Aut}(\pi_1(V,\star))$. By [Lu78, Cor. 2.2], $\hat{\mathcal{T}}$ coincides with the subgroup $\hat{\mathcal{T}}_\circ$ of $\hat{\mathcal{H}}$ generated by disk-twists. There is a short exact sequence

$$1 \to \mathbb{Z} \longrightarrow \mathcal{M} \xrightarrow{p} \hat{\mathcal{M}} \to 1, \tag{5.1}$$

where $1 \in \mathbb{Z}$ is mapped to the Dehn twist T_ζ along the boundary curve $\zeta = \partial\Sigma$, and p is the canonical map. Let $f \in \mathcal{T}$. Clearly $p(f) \in \hat{\mathcal{T}}$ so that $p(f) \in \hat{\mathcal{T}}_\circ$. Thus, for some $h \in \mathcal{T}_\circ$ we have $p(h) = p(f)$. Hence $f = h\,T_\zeta^n$ for some $n \in \mathbb{Z}$. Since T_ζ is a disk-twist, we have $f \in \mathcal{T}_\circ$. □

We regard $\mathcal{H}$ and $\mathcal{T}$ as subgroups of the automorphism group $\mathrm{Aut}(\pi)$ of the free group $\pi := \pi_1(\Sigma, \star)$, via the Dehn–Nielsen representation $\mathcal{M} \to \mathrm{Aut}(\pi)$. Set $F := \pi_1(V, \star)$ and let $\varpi : \pi \to F$ be induced by the inclusion $\iota : \Sigma \hookrightarrow V$. Then, for $\mathsf{A} := \ker \varpi$, we have the free pair (π, A) and we can consider the subgroup $\mathcal{G} := \mathrm{Aut}(\pi, \mathsf{A})$ of $\mathrm{Aut}(\pi)$. Note that A is isomorphic to the relative homotopy group $\pi_2(V, \Sigma)$.

Theorem 5.2 (Griffiths)**.** *We have $\mathcal{H} = \mathcal{M} \cap \mathcal{G}$.*

Proof. This is derived from Griffiths' theorem [Gri64]. Here we use the notations in the proof of Theorem 5.1. The inclusion $\mathcal{H} \subset \mathcal{M} \cap \mathcal{G}$ follows easily from the functoriality of the fundamental group.

To prove the converse inclusion, let $f \in \mathcal{M} \cap \mathcal{G}$ and $\hat{f} = p(f) \in \hat{\mathcal{M}}$. As an automorphism of $\pi_1(\partial V, \star)$, $\hat{f}$ preserves the kernel of $\iota_* : \pi_1(\partial V, \star) \to \pi_1(V, \star)$. Thus we have $\hat{f} \in \hat{\mathcal{H}}$ by [Gri64, Cor. 10.2]. Hence for some $h \in \mathcal{H}$ we have $p(h) = \hat{f}$. By the short exact sequence (5.1), we have $f = h\, T_\zeta^n$ for some $n \in \mathbb{Z}$, hence $f \in \mathcal{H}$. □

5.2. **The Johnson filtration of $\mathcal{H}$.** By Theorem 5.2 we can apply to $\mathcal{H}$ the constructions and results of the previous sections for $\mathcal{G} = \mathrm{Aut}(\pi, \mathsf{A})$.

In particular, by restricting the filtrations (3.3) of $\mathcal{G}$ to $\mathcal{H}$, and setting $\mathcal{H}_m = \mathcal{H} \cap \mathcal{G}_m$ and $\mathcal{H}_m^0 = \mathcal{H} \cap \mathcal{G}_m^0$ for $m \geq 0$, we obtain two nested filtrations

$$\mathcal{H} = \mathcal{H}_0^0 = \mathcal{H}_0 \geq \mathcal{H}_1^0 \geq \mathcal{H}_1 \geq \cdots \geq \mathcal{H}_{m-1} \geq \mathcal{H}_m^0 \geq \mathcal{H}_m \geq \cdots \tag{5.2}$$

such that

$$\bigcap_{m \geq 0} \mathcal{H}_m^0 = \bigcap_{m \geq 0} \mathcal{H}_m = \{1\}. \tag{5.3}$$

It turns out that these two filtrations coincide.

Theorem 5.3. *For each $m \geq 0$, we have $\mathcal{H}_m^0 = \mathcal{H}_m$.*

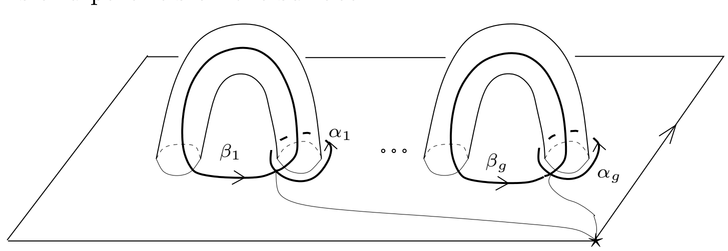
To prove Theorem 5.3, we need the identification of $\mathcal{M}$ with the subgroup of $\mathrm{Aut}(\pi)$ fixing the homotopy class

$$\zeta := [\partial \Sigma]$$

of the boundary curve. We write ζ in an explicit basis of the free group π as follows. Let $g \geq 1$ be the genus of Σ, and fix a system

$$(\alpha, \beta) = (\alpha_1, \ldots, \alpha_g, \beta_1, \ldots, \beta_g) \tag{5.4}$$

of meridians and parallels on the surface Σ:



Here the curves $\alpha_1, \ldots, \alpha_g$ bound pairwise-disjoint embedded disks in V. The basis of π defined by (α, β) and the connecting arcs to $\star$ shown above is still denoted by

(α, β). Then we have

$$\zeta^{-1} = \prod_{i=1}^{g} \left[\beta_i^{-1}, \alpha_i\right]. \tag{5.5}$$

Proof of Theorem 5.3. It suffices to prove $\mathcal{H}_m^0 \subset \mathcal{H}_m^1$. Thus, for $f \in \mathcal{H}_m^0 = \mathcal{H} \cap \mathcal{G}_m^0$, we need to check that

$$f(a)a^{-1} \in \mathsf{A}_{m+1} \quad \text{for all } a \in \mathsf{A}. \tag{5.6}$$

Since $f \in \mathcal{G}_m^0$ and $\mathsf{A} = \langle\langle \alpha_1, \ldots, \alpha_g \rangle\rangle$, it suffices to verify (5.6) for $a = \alpha_i$ with $i = 1, \ldots, g$. Setting

$$u_i := f(\alpha_i)\alpha_i^{-1} \in \mathsf{A}_m, \quad v_i := f(\beta_i)\beta_i^{-1} \in \mathsf{A}_m, \quad (i = 1, \ldots, g),$$

we have

$$\begin{aligned} f([\alpha_i, \beta_i^{-1}]) &= [f(\alpha_i), f(\beta_i)^{-1}] = [u_i\alpha_i, \beta_i^{-1}v_i^{-1}] = [u_i\alpha_i, \beta_i^{-1}] \cdot [u_i\alpha_i, v_i^{-1}]^{\beta_i} \\ &\underset{\mathsf{A}_{m+1}}{\equiv} [u_i\alpha_i, \beta_i^{-1}] = {}^{u_i}[\alpha_i, \beta_i^{-1}] \cdot [u_i, \beta_i^{-1}] \underset{\mathsf{A}_{m+1}}{\equiv} [\alpha_i, \beta_i^{-1}] \cdot [u_i, \beta_i^{-1}]. \end{aligned}$$

Hence, by (5.5), we get

$$\begin{aligned} f(\zeta^{-1}) = f\left(\prod_{i=1}^{g}[\beta_i^{-1}, \alpha_i]\right) &\underset{\mathsf{A}_{m+1}}{\equiv} \prod_{i=1}^{g}[\beta_i^{-1}, u_i] \cdot [\beta_i^{-1}, \alpha_i] \\ &\underset{\mathsf{A}_{m+1}}{\equiv} \left(\prod_{i=1}^{g}[\beta_i^{-1}, \alpha_i]\right) \cdot \left(\prod_{i=1}^{g}[\beta_i^{-1}, u_i]\right) = \zeta^{-1} \cdot \prod_{i=1}^{g}[\beta_i^{-1}, u_i]. \end{aligned}$$

It follows that

$$1 \underset{\mathsf{A}_{m+1}}{\equiv} \prod_{i=1}^{g}[\beta_i^{-1}, u_i] = \prod_{i=1}^{g} {u_i}^{\beta_i} \cdot u_i^{-1}.$$

Thus, we obtain

$$\sum_{i=1}^{g} \left(x_i^{-1} - 1\right)[u_i]_m = 0 \in \overline{\mathsf{A}}_m,$$

where $x_i = [\beta_i] \in F = \pi/\mathsf{A}$ and we use the $\mathbb{Z}[F]$-module structure of $\overline{\mathsf{A}}_m$. Since the free group F is left-orderable, we can apply Lemma 5.5 below to deduce that the $\mathbb{Z}[F]$-module $\overline{\mathsf{A}}_m = \mathrm{Lie}_m(\mathbb{A})$ is free. Then, it follows from Lemma 5.6 below that $[u_i]_m = 0 \in \overline{\mathsf{A}}_m$ for all i, i.e., $u_i \in \mathsf{A}_{m+1}$ for all i. □

The rest of this section is devoted to some lemmas used in the proof of Theorem 5.3. We shall need the following definitions.

The free magma $\mathrm{Mag}(S)$ on a set S consists of non-associative words in the alphabet S. Let $|w|$ denote the length of such a word w. For instance, if $x, y \in S$, then $(x, ((x, y), y)) \in \mathrm{Mag}(S)$ and $|(x, ((x, y), y))| = 4$. A *Hall set* on the alphabet S [Reu93, §4.1] is a totally-ordered subset $H \subset \mathrm{Mag}(S)$ containing S and satisfying the following two conditions:

(H_1) for any word $h = (h', h'')$ in $H \setminus S$, we have $h'' \in H$ and $h < h''$;

(H_2) for any word $h = (h', h'')$ in $\mathrm{Mag}(S) \setminus S$, we have $h \in H$ if and only if

$$h', h'' \in H \text{ and } h' < h'' \text{ and either } h' \in S \text{ or } h' = (u, v) \text{ with } v \geq h''.$$

Note that, if a group G acts on a set S, then it also acts on $\mathrm{Mag}(S)$ by acting on every letter of any word. For instance, if $x, y \in S$ and $g \in G$, then $g \cdot (x,(y,x)) = (g \cdot x,(g \cdot y, g \cdot x))$.

Lemma 5.4. *Let G be a group acting on a set S. Let $\leq$ be a total order on S such that $s \leq t$ implies $g \cdot s \leq g \cdot t$ for all $s, t \in S$ and $g \in G$. Then, there exists a G-stable Hall set H on the alphabet S such that the order $\leq$ of H extends that of S.*

Proof. We shall prove the lemma by refining the usual argument for the existence of Hall sets (see e.g. [Reu93, Prop. 4.1]).

Let $\mathrm{Mag}(\bullet)$ denote the free magma on one element $\bullet$. The unique map $S \to \{\bullet\}$ induces a magma homomorphism $p : \mathrm{Mag}(S) \to \mathrm{Mag}(\bullet)$, which records the parenthesization of non-associative words in S. For any $u \in \mathrm{Mag}(\bullet)$, the fiber $p^{-1}(u)$ can be canonically identified with $S^{|u|}$ (for instance, given $u = (\bullet,(\bullet,\bullet))$, we identify the word $(s_1,(s_2,s_3))$ with the triplet (s_1,s_2,s_3) for any $s_1,s_2,s_3 \in S$). Choose a total order of $\mathrm{Mag}(\bullet)$ such that

$$\text{for all } u,u' \in \mathrm{Mag}(\bullet),\ |u| < |u'| \text{ implies } u > u'. \tag{5.7}$$

It lifts via p to a unique total order of $\mathrm{Mag}(S)$ that restricts to the lexicographic order of every fiber $p^{-1}(u) \simeq S^{|u|}$. Since the order of S is compatible with the G-action, so is this total order of $\mathrm{Mag}(S)$.

Then, the condition (H_2) gives an inductive rule to construct a Hall set H starting with S in length 1 (the order of H is then the restriction of the total order of $\mathrm{Mag}(S)$). Then (H_1) follows from (5.7).

It remains to verify that the Hall set H is G-stable. Let $h \in H$ and $g \in G$. One verifies $g \cdot h \in H$ by induction on $|h|$. If $|h| = 1$, then (obviously) $h \in S$ so that $g \cdot h \in S \subset H$. If $|h| > 1$, then $h = (h',h'')$ satisfies (H_2) and, using the compatibility of the G-action with the total order $\leq$ in $\mathrm{Mag}(S)$, it is straightforward to verify that $g \cdot h = (g \cdot h', g \cdot h'')$ also satisfies (H_2). □

Lemma 5.5. *Let $(G,\leq)$ be a left-ordered group and M a free $\mathbb{Z}[G]$-module. Then,* $\mathrm{Lie}(M)$ *is free as a $\mathbb{Z}[G]$-module.*

Proof. Let X be a $\mathbb{Z}[G]$-basis of M, and $\leq$ a total order on X. Then

$$G \cdot X = \{ g \cdot x \,|\, g \in G, x \in X \}$$

is a $\mathbb{Z}$-basis of M. Identifying $G \cdot X$ with $X \times G$ in the obvious way, we can transport the lexicographic order of the latter to the former. Thus, $G \cdot X$ is a totally ordered G-set whose order is compatible with the G-action. Hence, by Lemma 5.4, there exists a G-stable Hall set $H \subset \mathrm{Mag}(G \cdot X)$. Let $\beta : \mathrm{Mag}(G \cdot X) \to \mathrm{Lie}(M)$ be the bracketing map. By a property of a Hall set (see e.g. [Reu93, Theorem 4.9]), $\beta(H)$ is a $\mathbb{Z}$-basis of $\mathrm{Lie}(M)$. Let E be the subset of H such that E retains, in each G-orbit contained in H, the unique non-associative word whose leftmost letter is in $X \subset G \cdot X$.

Let us verify that $\beta(E)$ freely generates the $\mathbb{Z}[G]$-module $\mathrm{Lie}(M)$. Since any element of H can be transformed to a (unique) element of E by the G-action, and since $\beta(H)$ generates $\mathrm{Lie}(M)$ as an abelian group, the subset $\beta(E)$ generates $\mathrm{Lie}(M)$ as a $\mathbb{Z}[G]$-module. Assume now a $\mathbb{Z}[G]$-linear relation between some elements of $\beta(E)$. Since the $\mathbb{Z}[G]$-module $\mathrm{Lie}(M)$ is graded, we can assume that this linear relation occurs in the homogeneous part $\mathrm{Lie}_m(M)$ of degree m for some $m \geq 1$:

$$\sum_{e \in E'_m} z_e \cdot \beta(e) \in \mathrm{Lie}_m(M),$$

where the sum is taken over a subset E'_m of E consisting of finitely many words of length m, and $z_e \in \mathbb{Z}[G]$ for all $e \in E'_m$. Decomposing $z_e = \sum_{g \in G} z_e(g) \cdot g$, we obtain a $\mathbb{Z}$-linear relation:

$$\sum_{e \in E'_m, g \in G} z_e(g) \cdot \beta(g \cdot e) \in \mathrm{Lie}_m(M)$$

Since $\beta(H)$ is $\mathbb{Z}$-free, we conclude that each $z_e(g) \in \mathbb{Z}$ is trivial, so that each $z_e \in \mathbb{Z}[G]$ is trivial. □

Lemma 5.6. *Let F be a free group of rank n with basis $\{x_1, \dots, x_n\}$, and let M be a free $\mathbb{Z}[F]$-module. If $m_1, \dots, m_n \in M$ satisfy*

$$\sum_{i=1}^{n} (1 - x_i) m_i = 0, \tag{5.8}$$

then $m_1 = \cdots = m_n = 0$.

Proof. We can reduce the lemma to the case where $M = \mathbb{Z}[F]$, by considering the coefficients with respect to a $\mathbb{Z}[F]$-basis of M. This case follows from the well-known fact that the augmentation ideal I_F of $\mathbb{Z}[F]$ is free on $x_1 - 1, \dots, x_n - 1$ as a $\mathbb{Z}[F]$-module. (See e.g. [Bro94, I.(4.4)].) □

6. First terms of the Johnson filtration for the handlebody group

In this section, we consider the first few terms of the Johnson filtration (5.2) of the handlebody group:

$$\mathcal{H} = \mathcal{H}_0 \ \geq \ \mathcal{H}_1 \ \geq \ \mathcal{H}_2.$$

Recall that the twist group $\mathcal{T} = \mathcal{H}_1^0$ is the subgroup of $\mathcal{H}$ acting trivially on $F \simeq \pi/\mathsf{A}$ or, equivalently, $\mathcal{T} = \mathcal{H}_1$ is the subgroup of $\mathcal{H}$ acting trivially on the abelianization $\mathbb{A}$ of A. Thus, $\mathcal{H}_0/\mathcal{H}_1$ embeds both into $\mathrm{Aut}(F)$ and $\mathrm{Aut}(\mathbb{A})$. Since any automorphism of F can be realized by an element of $\mathcal{H}$ (see [Lu78, Cor. 2.1], and also [Gri64, Zie61]), we have

$$\mathcal{H}_0/\mathcal{H}_1 \simeq \mathrm{Aut}(F). \tag{6.1}$$

The image of the embedding $\mathcal{H}_0/\mathcal{H}_1 \hookrightarrow \mathrm{Aut}(\mathbb{A})$ admits the following characterization. An element $\rho \in \mathrm{Aut}(\mathbb{A})$ is *quasi-equivariant* if there is a $\overrightarrow{\rho} \in \mathrm{Aut}(F)$ such that $\rho(f \cdot a) = \overrightarrow{\rho}(f) \cdot \rho(a)$ for all $f \in F$ and $a \in \mathbb{A}$. Clearly, quasi-equivariant elements form a subgroup $\mathrm{Aut}_{\mathrm{qe}}(\mathbb{A})$ of $\mathrm{Aut}(\mathbb{A})$. Since $\overrightarrow{\rho}$ is uniquely determined by ρ, there is a well-defined homomorphism

$$\overrightarrow{(-)} : \mathrm{Aut}_{\mathrm{qe}}(\mathbb{A}) \to \mathrm{Aut}\,(F).$$

Let $\mathrm{Aut}^{\zeta}_{\mathrm{qe}}(\mathbb{A})$ denote the subgroup of $\mathrm{Aut}_{\mathrm{qe}}(\mathbb{A})$ fixing $[\zeta] = [\zeta]_1 \in \mathbb{A} = \mathsf{A}_1/\mathsf{A}_2$. Having fixed a system of curves (α, β) as in (5.4), this element writes

$$[\zeta] = \sum_{i=1}^{g} (1 - x_i^{-1}) \cdot a_i, \tag{6.2}$$

where $a_i = [\alpha_i] \in \mathbb{A}$ and $x_i = \varpi(\beta_i) \in F$. In the sequel, for any matrix $M = (m_{ij})_{i,j} \in \mathrm{Mat}(g \times g; \mathbb{Z}[F])$, let $M^\dagger = (\overline{m_{ji}})_{i,j}$ denote its conjugate transpose.

Proposition 6.1. *The homomorphism* $\overrightarrow{(-)}$ *on* $\mathrm{Aut}_{\mathrm{qe}}(\mathbb{A})$ *induces an isomorphism*

$$\overrightarrow{(-)} : \mathrm{Aut}^{\zeta}_{\mathrm{qe}}(\mathbb{A}) \underset{\simeq}{\longrightarrow} \mathrm{Aut}(F),$$

which fits into the following commutative diagram

$$\begin{tikzcd}
 & \mathcal{H} \arrow[dl, two heads] \arrow[dr, two heads] \arrow[ddl, bend right=60, "\mathrm{Mag}_0^1"'] \arrow[ddr, bend left=60, "\mathrm{Mag}_0^0"] & \\
\mathrm{Aut}^{\zeta}_{\mathrm{qe}}(\mathbb{A}) \arrow[rr, "\overrightarrow{(-)}", "\simeq"'] \arrow[d, tail] & & \mathrm{Aut}(F) \arrow[d, tail, "J"'] \\
\mathrm{GL}(g;\mathbb{Z}[F]) \arrow[rr, "(-)^{\dagger,-1}", "\simeq"'] & & \mathrm{GL}(g;\mathbb{Z}[F])
\end{tikzcd}$$

where the left (resp. right) diagonal arrow gives the canonical action on $\mathbb{A}$ *(resp.* F*), the left vertical arrow maps any* $\rho \in \mathrm{Aut}^{\zeta}_{\mathrm{qe}}(\mathbb{A})$ *to the conjugate of its matrix* $\big(a_i^*(\rho(a_j))\big)_{i,j}$ *in the basis* $(a_1, \dots, a_g)$ *of* $\mathbb{A}$ *and the right vertical arrow* J *maps any* $r \in \mathrm{Aut}(F)$ *to its free Jacobian matrix* $J(r) = \Big(\frac{\partial r(x_j)}{\partial x_i}\Big)_{i,j}$ *in the basis* $(x_1, \dots, x_g)$*.*

Proof. The commutativity of the right upper triangle is the definition of Mag_0^0, that of the left upper triangle follows from Lemma 4.2 and that of the central triangle is clear. Hence, we only need to prove the commutativity of the bottom square:

$$\left(\overline{\frac{\partial \overrightarrow{\rho}(x_j)}{\partial x_i}}\right)^{-1}_{i,j} = \big(a_j^*(\rho(a_i))\big)_{i,j}, \quad \text{for all } \rho \in \mathrm{Aut}^{\zeta}_{\mathrm{qe}}(\mathbb{A}). \tag{6.3}$$

Note that

$$\rho([\zeta]) \overset{(6.2)}{=} -\sum_i \big(\overrightarrow{\rho}(x_i^{-1}) - 1\big) \cdot \rho(a_i) = -\sum_{i,l} (x_l^{-1} - 1) \overline{\frac{\partial \overrightarrow{\rho}(x_i)}{\partial x_l}} \cdot \rho(a_i)$$

which, using Lemma 5.6 and $\rho([\zeta]) = [\zeta]$, implies that

$$a_l = \sum_i \overline{\frac{\partial \overrightarrow{\rho}(x_i)}{\partial x_l}} \cdot \rho(a_i) = \sum_{i,k} \overline{\frac{\partial \overrightarrow{\rho}(x_i)}{\partial x_l}} a_k^*\big(\rho(a_i)\big) \cdot a_k. \tag{6.4}$$

Since $(a_1, \dots, a_g)$ is a $\mathbb{Z}[F]$-basis of $\mathbb{A}$, we obtain (6.3).

The surjectivity of $\mathcal{H} \to \mathrm{Aut}(F)$ implies that of $\overrightarrow{(-)}$. Injectivity of $\overrightarrow{(-)}$ follows from (6.4). The other injectivity and surjectivity in the diagram easily follow. □

Next, we would like to identify $\mathcal{H}_1/\mathcal{H}_2$. By Proposition 4.1, one can embed it into the abelian group $\mathrm{Mat}(g \times g; \mathbb{Z}[F])$ via the representation

$$\mathrm{Mag} := \mathrm{Mag}_1^0 : \mathcal{T} \longrightarrow \mathrm{Mat}(g \times g; \mathbb{Z}[F]), \ f \longmapsto \left(\varpi\Big(\overline{\frac{\partial f(\beta_j)}{\partial \alpha_i}}\Big)\right)_{i,j}.$$

The next proposition is a first step towards the determination of the image of Mag, and the more difficult problem of computing the abelianization of $\mathcal{T}$.

Proposition 6.2. *The Magnus representation takes values in hermitian matrices: for all $f \in \mathcal{T}$, we have $\mathrm{Mag}(f) = \mathrm{Mag}(f)^\dagger$. Besides, for all $f \in \mathcal{T}$ and $h \in \mathcal{H}$, we have*

$$\mathrm{Mag}(hfh^{-1}) = \mathrm{Mag}_0^0(h) \cdot h^F\big(\mathrm{Mag}(f)\big) \cdot \mathrm{Mag}_0^0(h)^\dagger, \tag{6.5}$$

where $h^F \in \mathrm{Aut}(F)$ is the action of h on $F = \pi_1(V, \star)$.

Proof. Set $n = 2g$ and $(z_1, \dots, z_n) = (\alpha_1, \dots, \alpha_g, \beta_1, \dots, \beta_g)$. Let $f \in \mathcal{M}$. We start by recalling that the condition for $f \in \mathrm{Aut}(\pi)$ to preserve the homotopy intersection form η (see §A.1) implies some strong conditions on the free Jacobian matrix

$$J(f) = \left(\overline{\frac{\partial f(z_j)}{\partial z_i}}\right)_{i,j} \in \mathrm{GL}(2g; \mathbb{Z}[\pi]).$$

(These appear under equivalent forms e.g. in [Mo93] and [Pe06].)

Recall that the (left) Fox derivatives $\frac{\partial}{\partial z_i}$ are uniquely defined by (4.1) and, similarly, we define some (right) Fox derivatives $\frac{\text{\reflectbox{$\partial$}}}{\text{\reflectbox{$\partial$}} z_i}$ by the identity

$$w - \varepsilon(w) = \sum_{i=1}^n (z_i - 1) \frac{\text{\reflectbox{∂}} w}{\text{\reflectbox{∂}} z_i} \quad \text{for all } w \in \mathbb{Z}[\pi].$$

The properties (A.2)–(A.3) of η to be a Fox pairing imply that

$$\eta(x, y) = \sum_{i,j} \frac{\partial x}{\partial z_i} \eta(z_i, z_j) \frac{\text{\reflectbox{∂}} y}{\text{\reflectbox{∂}} z_j} \quad \text{for all } x, y \in \mathbb{Z}[\pi]. \tag{6.6}$$

Using (6.6), the identity $f \circ \eta = \eta \circ (f \times f)$ translates into the matrix identity:

$$f(E) = \left(\frac{\partial f(z_i)}{\partial z_j}\right)_{i,j} \cdot E \cdot \left(\frac{\text{\reflectbox{∂}} f(z_j)}{\text{\reflectbox{∂}} z_i}\right)_{i,j},$$

where E denotes the matrix of η in the basis $(z_1, \dots, z_n)$. It easily follows from the definitions of left and right Fox derivatives that $\frac{\text{\reflectbox{$\partial$}} w}{\text{\reflectbox{$\partial$}} z_i} = z_i^{-1} \overline{\frac{\partial w}{\partial z_i}} w$ for any $w \in \pi$. Hence we obtain

$$f(E) = J(f)^\dagger \cdot E \cdot \mathrm{diag}(z_1^{-1}, \dots, z_n^{-1}) \cdot J(f) \cdot \mathrm{diag}(f(z_1), \dots, f(z_n)). \tag{6.7}$$

Assume now that $f \in \mathcal{T}$. By applying $\varpi : \mathbb{Z}[\pi] \to \mathbb{Z}[F]$, the previous matrix identity simplifies to

$$\varpi(f(E)) = \varpi(E) = J^F(f)^\dagger \cdot \varpi(E) \cdot (I \oplus D^{-1}) \cdot J^F(f) \cdot (I \oplus D), \tag{6.8}$$

where $I = I_g$ is the identity matrix and $D = \mathrm{diag}(x_1, \dots, x_g)$ is the diagonal matrix with entries x_i. It also follows from Proposition 4.1 that

$$J^F(f) = \left(\varpi\Big(\overline{\frac{\partial f(z_j)}{\partial z_i}}\Big)\right)_{i,j} = \left(\begin{array}{c|c} I & \mathrm{Mag}(f) \\ \hline 0 & I \end{array}\right) \tag{6.9}$$

and from the computation of E in §A.1 that

$$\varpi(E) = \left(\begin{array}{c|c} 0 & D \\ \hline -I & D - I \end{array}\right).$$

Then the identity $\mathrm{Mag}(f) = \mathrm{Mag}(f)^\dagger$ easily follows from (6.8).

Let also $h \in \mathcal{H}$. Since J^F is a crossed homomorphism, we get

$$J^F(hfh^{-1}) \overset{(4.3)}{=} J^F(h) \cdot h^F\big(J^F(f)\big) \cdot h^F\big(J^F(h^{-1})\big),$$

where $h^F \in \mathrm{Aut}(F)$ is the action of h on $F = \pi_1(V,\star)$. Then, Propositions 4.1 and 6.1 give

$$J^F(h) = \left(\begin{array}{c|c} \mathrm{Mag}_0^0(h) & \mathrm{Mag}_1^0(h) \\ \hline 0 & \mathrm{Mag}_0^0(h)^{\dagger,-1} \end{array}\right).$$

It is now straightforward to deduce (6.5) from (6.9) and the two identities above. □

Remark 6.3. By applying (6.7) to an $f \in \mathcal{H}$, we get an alternative justification for the identity $\mathrm{Mag}_0^1(f) \cdot \mathrm{Mag}_0^0(f)^\dagger = I \in \mathrm{GL}(g;\mathbb{Z}[F])$, which is contained in Proposition 6.1.

Example 6.4. Let $T := T_{\partial\Sigma}$ be the Dehn twist along the boundary curve. Then we have

$$\varpi\Big(\frac{\partial T(\beta_i)}{\partial \alpha_j}\Big) = \varpi\Big(\frac{\partial\, {}^{\zeta}\beta_i}{\partial \alpha_j}\Big) = (1-x_i)\,\varpi\Big(\frac{\partial \zeta}{\partial \alpha_j}\Big) \overset{(6.2)}{=} (1-x_i)\,(1-x_j^{-1}). \tag{6.10}$$

Hence we have $\mathrm{Mag}(T) = \big((1-x_i)(1-x_j^{-1})\big)_{i,j}$.

7. Johnson homomorphisms for the handlebody group

Restricting (3.12) to $\mathcal{H} = \mathcal{H}_0$ yields homomorphisms

$$\tau_0^0 : \mathcal{H} \longrightarrow \mathrm{Aut}(F), \quad \tau_0^1 : \mathcal{H} \longrightarrow \mathrm{Aut}\,\big(\mathbb{A}\big),$$

which satisfy (3.15), and whose images are described in Proposition 6.1. Furthermore, restricting (3.13) yields homomorphisms

$$\tau_m^0 : \mathcal{H}_m \longrightarrow Z^1\big(F, \overline{\mathsf{A}}_m\big), \quad \tau_m^1 : \mathcal{H}_m \longrightarrow \mathrm{Hom}\,\big(\mathbb{A}, \overline{\mathsf{A}}_{m+1}\big) \quad (m \geq 1),$$

which satisfy (3.16). These maps satisfy (3.17)–(3.20). By (3.14) we have

$$\ker \tau_m^0 = \mathcal{H}_{m+1} \quad \text{and} \quad \ker \tau_m^1 = \mathcal{H}_{m+1}. \tag{7.1}$$

Example 7.1. By Proposition 4.1, in degree $m = 1$, $\tau_1^0 : \mathcal{T} \to Z^1(F,\mathbb{A})$ and $\tau_1^1 : \mathcal{T} \to \mathrm{Hom}(\mathbb{A}, \Lambda^2\mathbb{A})$ are equivalent to $\mathrm{Mag} = \mathrm{Mag}_1^0 : \mathcal{T} \to \mathrm{Mat}(g \times g; \mathbb{Z}[F])$, whose image is partly described in Proposition 6.2.

Equation (7.1) and Theorem 5.3 immediately imply the following.

Corollary 7.2. *The two families of Johnson homomorphisms $(\tau_m^0)_m$ and $(\tau_m^1)_m$ are equivalent to each other for the handlebody group.*

For some purposes (for instance, to have another viewpoint on Corollary 7.2), it will be also convenient to use the extended graded Lie algebra morphism

$$\overline{\tau}_\bullet : \overline{\mathcal{H}}_\bullet \longrightarrow \mathrm{Der}_\bullet(\overline{\mathsf{A}}_\bullet) \simeq D_\bullet(\overline{\mathsf{A}}_\bullet),$$

which encompasses the two families $(\tau_m^0)_m$ and $(\tau_m^1)_m$ into a single map. It follows from (7.1) that $\overline{\tau}_\bullet$ is injective. Clearly, $\overline{\tau}_\bullet$ takes values in the extended graded Lie subalgebra

$$\mathrm{Der}^\zeta_\bullet(\overline{\mathsf{A}}_\bullet) \simeq D^\zeta_\bullet(\overline{\mathsf{A}}_\bullet)$$

whose degree 0 part consists of the extended graded Lie algebra automorphisms of $\overline{\mathsf{A}}_\bullet$ that fix $[\zeta]_1 \in \overline{\mathsf{A}}_1$ and whose positive-degree part consists of extended graded Lie algebra derivations of $\overline{\mathsf{A}}_\bullet$ that vanish on $[\zeta]$. We call it the *extended graded Lie algebra of special derivations* of $\overline{\mathsf{A}}_\bullet$.

In the sequel, we will mainly focus on the twist group, for which it is enough to consider the morphism of graded Lie algebras

$$\overline{\tau}_+ : \overline{\mathcal{H}}_+ \longrightarrow \mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet) \simeq D^\zeta_+(\overline{\mathsf{A}}_\bullet). \tag{7.2}$$

Recall that $\overline{\tau}_m$ is equivariant in the sense that

$$\overline{\tau}_m([hth^{-1}]_m) = h_* \circ \overline{\tau}_m([t]_m) \circ h_*^{-1}$$

for any $m \geq 1$, $t \in \mathcal{H}_m$, $h \in \mathcal{H}$, where $h_* \in \mathrm{Aut}(\overline{\mathsf{A}}_\bullet)$ is the unique automorphism of extended graded Lie algebras given by $\tau_0^0(h) \in \mathrm{Aut}(F)$ in degree 0 and by $\tau_0^1(h) \in \mathrm{Aut}^\zeta_{\mathrm{qe}}(\mathbb{A})$ in degree 1.

The graded Lie algebra $\mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet) \simeq D^\zeta_+(\overline{\mathsf{A}}_\bullet)$ is a rich algebraic object, whose study is postponed to §8. In the meantime, we explain how the embedding (7.2) lifts to an embedding of $\mathcal{T} = \mathcal{H}_1$ into the degree-completion of $D^\zeta_+(\overline{\mathsf{A}}_\bullet)$. For this, we need the following refinement of Lemma 3.6.

Lemma 7.3. *There exists an expansion θ of the free pair (π, A) such that the associated map $\ell^\theta : \pi \to \widehat{\mathrm{Lie}}(\mathbb{A}^\mathbb{Q})$ satisfies*

$$\ell^\theta(\zeta) = [\zeta]_1 \in \mathbb{A}. \tag{7.3}$$

An expansion θ of (π, A) that satisfies the additional condition (7.3), i.e., $\ell^\theta(\zeta)$ is concentrated in degree 1, is called *special*. This is an analogue of the notion of symplectic expansion of π that was considered in relation with the classical study of Johnson homomorphisms for the Torelli group [Mas12]. (See Lemma 10.6 below, in this connection.)

Proof of Lemma 7.3. We start by recalling a related notion of special expansion for a free group with a given basis [AT12, Mas18]. Let D be a finitely-generated free group, with basis $(\delta_1, \dots, \delta_n)$. Let $\mathbb{D}^\mathbb{Q} := D_{\mathrm{ab}} \otimes \mathbb{Q}$ be its rational abelianization, and set $d_i := [\delta_i] \in \mathbb{D}^\mathbb{Q}$. A *special expansion* of D (relative to the basis $(\delta_1, \dots, \delta_n)$) is a monoid homomorphism $\theta_0 : D \to \widehat{T}(\mathbb{D}^\mathbb{Q})$ with the following two properties:

- for all $i \in \{1, \dots, n\}$, there exists a primitive element $v_i \in \widehat{T}(\mathbb{D}^\mathbb{Q})$ such that $\theta_0(\delta_i) = \exp(v_i)\exp(d_i)\exp(-v_i)$;
- we have $\theta_0(\delta_n \cdots \delta_2\delta_1) = \exp(d_1 + d_2 + \cdots + d_n)$.

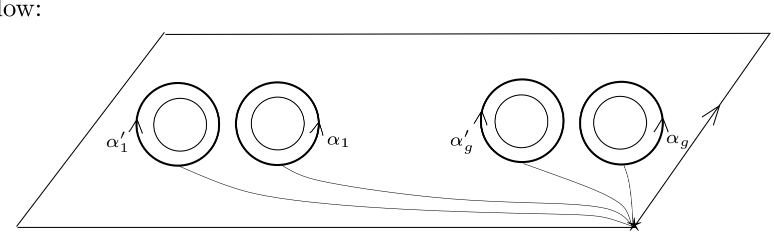
Such a map θ_0 can be constructed by successive finite-degree approximations of $v_1, \dots, v_n$. For instance, up to degree one, we can take

$$v_i = r_i d_i + \frac{1}{2}\sum_{i<j} d_j + (\deg \geq 2), \tag{7.4}$$

where $r_i \in \mathbb{Q}$ can be chosen arbitrarily.

Let (α, β) be a basis of π of type (5.4). Recall that the curves $\alpha_1, \dots, \alpha_g$ are meridians of V. Let $\Sigma' \subset \Sigma$ be the disk with $2g$ holes that is obtained from Σ by removing the g handles. Then $D := \pi_1(\Sigma', \star)$ is free on the loops $\alpha_1', \alpha_1, \dots, \alpha_g', \alpha_g$ shown below:

(7.5)



Let also B be the free group on $\beta_1, \dots, \beta_g$. Then

$$\pi \simeq \frac{D * B}{R}, \tag{7.6}$$

where R denotes the subgroup of the free product $D * B$ normally generated by the elements $\alpha'_i \beta_i^{-1} \alpha_i^{-1} \beta_i$ for all $i \in \{1, \dots, g\}$.

Choose now a special expansion $\theta_0 : D \to \widehat{T}(\mathbb{D}^{\mathbb{Q}})$ of the free group D (relative to the basis $\big((\alpha'_1)^{-1}, \alpha_1, \dots, (\alpha'_g)^{-1}, \alpha_g\big)$): thus, there exist primitive elements $u_1, u'_1, \dots, u_g, u'_g \in \widehat{T}(\mathbb{D}^{\mathbb{Q}})$ such that

$$\theta_0(\alpha_i) = \exp(u_i)\, \exp(a_i)\, \exp(-u_i), \quad \theta_0((\alpha'_i)^{-1}) = \exp(u'_i)\, \exp(-a'_i)\, \exp(-u'_i),$$

where $a'_i := [\alpha'_i] \in \mathbb{D}^{\mathbb{Q}}$ and $a_i := [\alpha_i] \in \mathbb{D}^{\mathbb{Q}}$, and the following condition is satisfied:

$$\theta_0\big(\alpha_g (\alpha'_g)^{-1} \cdots \alpha_1 (\alpha'_1)^{-1}\big) = \exp\big((a_1 - a'_1) + \cdots + (a_g - a'_g)\big) \tag{7.7}$$

The inclusion $\Sigma' \hookrightarrow \Sigma$ induces a homomorphism $D \to \mathsf{A}$ at the level of the fundamental groups, which further induces an (injective) algebra homomorphism $q : \widehat{T}(\mathbb{D}^{\mathbb{Q}}) \to \widehat{T}(\mathbb{A}^{\mathbb{Q}})$. Thus, we can define a multiplicative map $\theta_1 : D \to \widehat{T}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$ by

$$\theta_1(\alpha_i) := q\theta_0(\alpha_i) \otimes 1 \quad \text{and} \quad \theta_1(\alpha'_i) := q\theta_0(\alpha'_i) \otimes 1. \tag{7.8}$$

We also define a multiplicative map $\theta_2 : B \to \widehat{T}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$ by

$$\theta_2(\beta_i) := \exp\big(q(u_i)\big)\, \exp\big({}^{x_i} q(-u'_i)\big) \otimes x_i, \tag{7.9}$$

where $x_i = \varpi(\beta_i)$. Thus we obtain a multiplicative map

$$\theta_1 * \theta_2 : D * B \longrightarrow \widehat{T}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]. \tag{7.10}$$

For all $i \in \{1, \dots, g\}$, we have

$$\begin{aligned}
& \big(\theta_1 * \theta_2\big)\big(\alpha'_i \beta_i^{-1} \alpha_i^{-1} \beta_i\big) \\
= \;& \theta_1(\alpha'_i) \cdot \theta_2(\beta_i)^{-1} \cdot \theta_1(\alpha_i)^{-1} \cdot \theta_2(\beta_i) \\
= \;& \big(\exp q(u'_i)\, \exp q(a'_i)\, \exp q(-u'_i) \otimes 1\big) \cdot \big(\exp q(u'_i)\, \exp\big(q(-u_i)^{x_i}\big) \otimes x_i^{-1}\big) \\
& \cdot \big(\exp q(u_i)\, \exp q(-a_i)\, \exp q(-u_i) \otimes 1\big) \cdot \big(\exp q(u_i)\, \exp\big({}^{x_i} q(-u'_i)\big) \otimes x_i\big) \\
= \;& \big(\exp q(u'_i)\, \exp q(a'_i)\, \exp q\big((-u_i)^{x_i}\big) \otimes x_i^{-1}\big) \\
& \cdot \big(\exp q(u_i)\, \exp q(-a_i) \exp q\big({}^{x_i}(-u'_i)\big) \otimes x_i\big) \\
= \;& \exp q(u'_i)\, \exp q(a'_i)\, \exp q(-a_i)^{x_i} \exp q(-u'_i) \otimes 1 \;=\; 1 \otimes 1,
\end{aligned}$$

where the last identity follows from $q(a'_i) = q(a_i)^{x_i} \in \mathbb{A}^{\mathbb{Q}}$. It follows from (7.6) that $\theta_1 * \theta_2$ induces a multiplicative map

$$\theta : \pi \longrightarrow \widehat{T}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F].$$

That θ satisfies conditions (3.21) and (3.22) in Definition 3.5 follows directly from the definitions of θ_1 and θ_2. It remains to verify condition (7.3):

$$\begin{aligned}
\theta(\zeta) \overset{(5.5)}{=} \;& \theta\big([\alpha_g, \beta_g^{-1}] \cdots [\alpha_1, \beta_1^{-1}]\big) \\
= \;& \theta\big(\alpha_g (\alpha'_g)^{-1} \cdots \alpha_1 (\alpha'_1)^{-1}\big) \\
= \;& q\theta_0\big(\alpha_g (\alpha'_g)^{-1} \cdots \alpha_1 (\alpha'_1)^{-1}\big) \otimes 1 \\
\overset{(7.7)}{=} \;& q \exp\big((a_1 - a'_1) + \cdots + (a_g - a'_g)\big) \otimes 1 \\
= \;& \exp\big((q(a_1) - q(a'_1)) + \cdots + (q(a_g) - q(a'_g))\big) \otimes 1
\end{aligned}$$

$$= \quad \exp\big((q(a_1)-q(a_1)^{x_1})+\cdots+(q(a_g)-q(a_g)^{x_g})\big)\otimes 1 \overset{(6.2)}{=} \exp([\zeta]_1)\otimes 1.$$

□

Recall that the complete Lie algebra $\widehat{D}^{\zeta}_{+}\big(\overline{\mathsf{A}}^{\mathbb{Q}}_{\bullet}\big)$ can be viewed as a group whose multiplication is given by the BCH formula. The following provides an infinitesimal version of the action of $\mathcal{T}$ on the free pair (π,A).

Theorem 7.4. *Let θ be a special expansion of the free pair (π,A). There is a homomorphism*

$$\varrho^{\theta}:\mathcal{T}\longrightarrow \widehat{D}^{\zeta}_{+}\big(\overline{\mathsf{A}}^{\mathbb{Q}}_{\bullet}\big) \tag{7.11}$$

whose restriction to $\mathcal{H}_m$ $(m\geq 1)$ starts in degree m with (τ^0_m,τ^1_m) . Furthermore, ϱ^{θ} is injective.

Proof. This is obtained by restricting the homomorphism ϱ^{θ} of Theorem 3.7 to the twist group $\mathcal{T}=\mathcal{H}_1\subset\mathcal{G}_1$. Observe that, here, the condition for a $g\in\mathcal{T}$ to fix $\zeta\in\pi$ translates into the property for the derivation $\log(\rho^{\theta}(g))$ to vanish on $\theta(\zeta)$ or, equivalently, on $\log\theta(\zeta)=\ell^{\theta}(\zeta)$. □

8. The Lie algebra of special derivations for the handlebody group

In this section, we give two equivalent descriptions of the Lie algebra of special derivations $\mathrm{Der}^{\zeta}_{+}(\overline{\mathsf{A}}_{\bullet})\simeq D^{\zeta}_{+}(\overline{\mathsf{A}}_{\bullet})$.

8.1. **The graded Lie algebra D^0_+.** Let I_F be the augmentation ideal of $\mathbb{Z}[F]$, viewed as a left $\mathbb{Z}[F]$-module. So far, we have regarded $\mathbb{A}$ as a left $\mathbb{Z}[F]$-module using the left conjugation of π on A, but we can also regard it as a right $\mathbb{Z}[F]$-module $\mathbb{A}^r$ using the right conjugation. Given a left (resp. right) $\mathbb{Z}[F]$-module M, let $M^*=\mathrm{Hom}_{\mathbb{Z}[F]}(M,\mathbb{Z}[F])$ denote the module of $\mathbb{Z}[F]$-linear forms on M, which is a right (resp. left) $\mathbb{Z}[F]$-module. With these notations, the intersection operation $\langle -,-\rangle$ given in Proposition A.2 induces canonical isomorphisms

$$\mathbb{A}^r\simeq I_F^* \quad\text{and}\quad I_F\simeq(\mathbb{A}^r)^* \tag{8.1}$$

of right and left $\mathbb{Z}[F]$-modules, respectively.

Lemma 8.1. *For any left $\mathbb{Z}[F]$-module M, there is a canonical isomorphism*

$$\vartheta: Z^1(F,M)\xrightarrow{\simeq}\mathbb{A}^r\otimes_{\mathbb{Z}[F]}M.$$

Proof. For any $c\in Z^1(F,M)$, let $d:I_F\to M$ be the restriction to I_F of the $\mathbb{Z}$-linearization $c:\mathbb{Z}[F]\to M$ of c. Conversely, each $d\in\mathrm{Hom}_{\mathbb{Z}[F]}(I_F,M)$ yields a 1-cocycle $c\in Z^1(F,M)$ by $c(f)=d(f-1)$. Let ϑ be the composition of the following isomorphisms

$$Z^1(F,M)\simeq\mathrm{Hom}_{\mathbb{Z}[F]}\big(I_F,M\big)\simeq I_F^*\otimes_{\mathbb{Z}[F]}M \overset{(8.1)}{\simeq}\mathbb{A}^r\otimes_{\mathbb{Z}[F]}M.$$

□

Let $[-,-]:\mathbb{A}\times\overline{\mathsf{A}}_+\to\overline{\mathsf{A}}_+$ denote the restriction of the Lie bracket of $\overline{\mathsf{A}}_+$. We regard $\overline{\mathsf{A}}_+$ as a $\mathbb{Z}[F]$-module. Then we have $\overline{\mathsf{A}}_+/I_F\overline{\mathsf{A}}_+\simeq(\overline{\mathsf{A}}_+)_F$, the F-coinvariants of $\overline{\mathsf{A}}_+$. Define a $\mathbb{Z}$-linear map

$$\beta:\mathbb{A}^r\otimes_{\mathbb{Z}[F]}\overline{\mathsf{A}}_+\to\overline{\mathsf{A}}_+/I_F\overline{\mathsf{A}}_+$$

by composing $[-,-]$ with the projection $\overline{\mathsf{A}}_+\to\overline{\mathsf{A}}_+/I_F\overline{\mathsf{A}}_+$, and set

$$D^0_+=\big\{c\in Z^1(F,\overline{\mathsf{A}}_+):\beta\vartheta(c)=0\big\}. \tag{8.2}$$

The following proposition means that every element of $\mathrm{Der}^{\zeta}_{+}(\overline{\mathsf{A}}_\bullet)$ is determined by its degree 0 part.

Proposition 8.2. *We have an isomorphism*

$$\mathrm{Der}^{\zeta}_{+}(\overline{\mathsf{A}}_\bullet) \xrightarrow{\simeq} D^0_+,\ (d_i)_{i\geq 0} \longmapsto d_0, \tag{8.3}$$

Proof. We first verify that, for any $(d_i)_{i\geq 0} \in \mathrm{Der}_{+}(\overline{\mathsf{A}}_\bullet)$ with $d_1([\zeta]) = 0$ we have $\beta\vartheta(d_0) = 0$. This follows from

$$\beta\vartheta(d_0) \equiv d_1([\zeta]) \mod I_F\overline{\mathsf{A}}_+, \tag{8.4}$$

which we now prove. As in (6.2), let $a_i = [\alpha_i] \in \overline{\mathsf{A}}_1 = \mathbb{A}$ and $x_i = [\beta_i] \in \overline{\mathsf{A}}_0 \simeq F$, for $i \in \{1,\dots,g\}$. By (A.17), the isomorphism (8.1) maps the dual basis $\big((x_i-1)^*\big)_i$ of I_F^* to -1 times the basis $(a_i)_i$ of $\mathbb{A}^r$. Therefore,

$$\beta\vartheta(d_0) = \beta\Big(-\sum_{i=1}^{g} a_i\otimes d_0(x_i)\Big) \equiv -\sum_{i=1}^{g}[a_i, d_0(x_i)] \mod I_F\overline{\mathsf{A}}_+. \tag{8.5}$$

On the other hand, we have

$$\begin{aligned} d_1([\zeta]) &\overset{(6.2)}{=} d_1\big(\sum_{i=1}^{g}(1-x_i^{-1})\cdot a_i\big) \\ &\overset{(3.7)}{=} \sum_{i=1}^{g}(1-x_i^{-1})\cdot d_1(a_i) - \sum_{i=1}^{g}[d_0(x_i^{-1}), x_i^{-1}\cdot a_i] \\ &= \sum_{i=1}^{g}(1-x_i^{-1})\cdot d_1(a_i) + \sum_{i=1}^{g}x_i^{-1}[d_0(x_i), a_i] \end{aligned} \tag{8.6}$$

which immediately implies (8.4).

Next, we prove the injectivity of (8.3). Let $(d_i)_{i\geq 0} \in \mathrm{Der}^{\zeta}_{+}(\overline{\mathsf{A}}_\bullet)$ with $d_0 = 0$. We deduce from (8.6) that

$$\sum_{i=1}^{g}(1-x_i^{-1})\cdot d_1(a_i) = 0$$

and, by Lemmas 5.5 and 5.6, we obtain $d_1(a_1) = \cdots = d_1(a_g) = 0$. Therefore d_1 and consequently $(d_i)_{i\geq 0}$ are trivial.

Finally, we prove the surjectivity of (8.3). Let $c \in D^0_+$. It follows from (8.5) that $\sum_{i=1}^{g} x_i^{-1}\cdot[a_i, c(x_i)] \in I_F\overline{\mathsf{A}}_+$. Hence, for some $u_1,\dots,u_g \in \overline{\mathsf{A}}_+$ we have

$$\sum_{i=1}^{g} x_i^{-1}[a_i, c(x_i)] = \sum_{i=1}^{g}(1-x_i^{-1})\cdot u_i. \tag{8.7}$$

Since the abelian group $\mathbb{A}$ is free on the ${}^f a_i$ for all $f \in F$ and $i \in \{1,\dots,g\}$, there is a unique homomorphism $u : \mathbb{A} \to \overline{\mathsf{A}}_+$ such that

$$u({}^f a_i) = {}^f u_i + \big[c(f), {}^f a_i\big].$$

By construction, the pair (c,u) belongs to $D_+(\overline{\mathsf{A}}_\bullet)$ and, setting $(d_0,d_1) = (c,u)$, it can be extended to $(d_i)_{i\geq 0} \in \mathrm{Der}_{+}(\overline{\mathsf{A}}_\bullet)$. Then, combining (8.6) and (8.7), we get $d_1([\zeta]) = 0$. Therefore, there exists a $(d_i)_{i\geq 0} \in \mathrm{Der}^{\zeta}_{+}(\overline{\mathsf{A}}_\bullet)$ such that $d_0 = c$. ☐

Remark 8.3. According to (3.8), the Lie bracket in D^0_+ corresponding to the Lie bracket of derivations through (8.3) is given by the following formula. For any $d, e \in D^0_+$, we define $[d,e]$ by

$$[d,e](f) = d_+(e(f)) - e_+(d(f)) - [d(f), e(f)] \quad \text{for all } f \in F, \tag{8.8}$$

where d_+ and e_+ are the derivations of $\mathrm{Lie}(\mathbb{A}) = \overline{\mathsf{A}}_+$ completing d and e, respectively, to derivations of the extended graded Lie algebra $\overline{\mathsf{A}}_\bullet$.

Proposition 8.6 below describes the map $D^0_+ \to \mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet)$ inverse to (8.3). This allows for a complete understanding of the bracket (8.8).

8.2. **The graded Lie algebra D^1_+.** The group F acts on the abelian group $\mathrm{Hom}(\mathbb{A}, \overline{\mathsf{A}}_+)$ by the rule

$$({}^f d)(a) := {}^f\big(d({}^{f^{-1}}a)\big) \quad \text{for all } a \in \mathbb{A}$$

for any $d \in \mathrm{Hom}(\mathbb{A}, \overline{\mathsf{A}}_+)$ and $f \in F$. An element $d \in \mathrm{Hom}(\mathbb{A}, \overline{\mathsf{A}}_+)$ is said to be *quasi-equivariant* if, for all $f \in F$, we have ${}^f d - d = [v, -]$ for some $v \in \overline{\mathsf{A}}_+$. Set

$$D^1_+ = \big\{ d \in \mathrm{Hom}(\mathbb{A}, \overline{\mathsf{A}}_+) : d \text{ is quasi-equivariant with values in } \overline{\mathsf{A}}_{\geq 2} \text{ and } d([\zeta]) = 0 \big\}.$$

The following proposition means that every element of $\mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet)$ is also determined by its degree 1 part.

Proposition 8.4. *We have an isomorphism*

$$\mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet) \xrightarrow{\simeq} D^1_+, \ (d_i)_{i\geq 0} \longmapsto d_1. \tag{8.9}$$

Proof. For $(d_i)_{i\geq 0} \in \mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet)$, the quasi-equivariance of d_1 follows from (3.7).

We prove the injectivity. Let $(d_i)_{i\geq 0} \in \mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet)$ with $d_1 = 0$. Let $f \in F$. By (3.7), $d_0(f)$ commutes with $\mathbb{A} = \overline{\mathsf{A}}_1$ in the free Lie algebra $\mathrm{Lie}(\mathbb{A}) = \overline{\mathsf{A}}_+$, hence $d_0(f) = 0$. Thus, d_0 and consequently $(d_i)_{i\geq 0}$ are trivial.

We now prove the surjectivity. Let $d_1 \in D^1_+$. There exists a (unique) map $d_0 : F \to \overline{\mathsf{A}}_+$ such that $[d_0(f), -] = d_1 - {}^f d_1$ for any $f \in F$, and it is easily checked that d_0 is a 1-cocycle. By construction, we have $(d_0, d_1) \in D^\zeta_+(\overline{\mathsf{A}}_\bullet)$, which extends to a derivation $(d_i)_{i\geq 0} \in \mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet)$. □

Remark 8.5. According to (3.9), the Lie bracket in D^1_+ corresponding to the Lie bracket of derivations through (8.9) is given by the following formula. For any $d, e \in D^1_+$, define $[d,e]$ by

$$[d,e](a) = d_+(e(a)) - e_+(d(a)) \quad \text{for all } a \in \mathbb{A},$$

where d_+ and e_+ are the derivations of $\mathrm{Lie}(\mathbb{A}) = \overline{\mathsf{A}}_+$ extending d and e respectively.

The following proposition describes the isomorphism $D^0_+ \simeq D^1_+$ that is obtained by combining Propositions 8.2 and 8.4.

Proposition 8.6. *The* 1*-cocycle* $c : F \to \mathrm{Lie}(\mathbb{A})$ *in* D^0_+ *corresponding to a homomorphism* $d : \mathbb{A} \to \mathrm{Lie}(\mathbb{A})$ *in* D^1_+ *is given by*

$$[c(f), -] = d - {}^f d \quad \textit{for all } f \in F. \tag{8.10}$$

Conversely, the homomorphism $d : \mathbb{A} \to \mathrm{Lie}(\mathbb{A})$ *in* D^1_+ *corresponding to a* 1*-cocycle* $c : F \to \mathrm{Lie}(\mathbb{A})$ *in* D^0_+ *is given by*

$$d(a) = -\Big[\overline{\Psi\big(\vartheta(c)^\ell, a\big)^\ell \cdot \vartheta(c)^r, \Psi\big(\vartheta(c)^\ell, a\big)^r}\Big] \quad \textit{for all } a \in \mathbb{A}, \tag{8.11}$$

where $\vartheta(c)^\ell \otimes \vartheta(c)^r \in \mathbb{A} \otimes \mathrm{Lie}(\mathbb{A})$ *denotes a lift of* $\vartheta(c) \in \mathbb{A}^r \otimes_{\mathbb{Z}[F]} \mathrm{Lie}(\mathbb{A})$ *such that* $[\vartheta(c)^\ell, \vartheta(c)^r] = 0 \in \mathrm{Lie}(\mathbb{A})$.

In the above proposition, $\Psi : \mathbb{A} \otimes \mathbb{A} \to \mathbb{Z}[F] \otimes \mathbb{A}$ is the intersection operation introduced in §A.4. Recall also that, with our conventions, the expansion of a tensor product $\Psi(a, b) \in \mathbb{Z}[F] \otimes \mathbb{A}$ is denoted by $\Psi(a, b)^\ell \otimes \Psi(a, b)^r$.

Proof of Proposition 8.6. The first statement follows immediately from the proof of Proposition 8.4.

To prove the second statement, let $c \in D^0_+$ and let us first check that $\vartheta(c) \in \mathbb{A}^r \otimes_{\mathbb{Z}[F]} \mathrm{Lie}(\mathbb{A})$ does have a lift to $\mathbb{A} \otimes \mathrm{Lie}(\mathbb{A})$ with trivial Lie bracket. Choose any lift $\sum_i u_i \otimes v_i \in \mathbb{A} \otimes \mathrm{Lie}(\mathbb{A})$ of $\vartheta(c)$. Since $\beta\vartheta(c) = 0$, there exist some $f_j \in F$ and $w_j \in \mathrm{Lie}(\mathbb{A})$ such that

$$\sum_i [u_i, v_i] = \sum_j (f_j - 1) \cdot w_j.$$

For every j, we can find some $s_{jk} \in \mathbb{A}$ and $t_{jk} \in \mathrm{Lie}(\mathbb{A})$ such that $w_j = \sum_k [s_{jk}, t_{jk}]$. Hence

$$\sum_i u_i \otimes v_i - \sum_{j,k} (f_j \cdot s_{jk}) \otimes (f_j \cdot t_{jk}) + \sum_{j,k} s_{jk} \otimes t_{jk}$$

has trivial Lie bracket and, clearly, it is also a lift of $\vartheta(c)$.

Let now $d : \mathbb{A} \to \mathrm{Lie}(\mathbb{A})$ be the homomorphism defined by (8.11). The condition on the lift $\vartheta(c)^\ell \otimes \vartheta(c)^r$ of $\vartheta(c)$ implies that

$$d([\zeta]) \overset{(A.26)}{=} -[\vartheta(c)^r, \vartheta(c)^\ell] = 0.$$

Besides, for any $f \in F$ and $a \in \mathbb{A}$, we have

$$\begin{aligned} d({}^f a) &= -\Big[\overline{\Psi\big(\vartheta(c)^\ell, {}^f a\big)^\ell} \cdot \vartheta(c)^r, \Psi\big(\vartheta(c)^\ell, {}^f a\big)^r\Big] \\ &\overset{(A.28)}{=} -\Big[\overline{\Psi\big(\vartheta(c)^\ell, a\big)^\ell f^{-1}} \cdot \vartheta(c)^r, f \cdot \Psi\big(\vartheta(c)^\ell, a\big)^r\Big] + \big[\langle f, \vartheta(c)^\ell \rangle \cdot \vartheta(c)^r, {}^f a\big] \\ &= {}^f d(a) + \big[c(f), {}^f a\big]. \end{aligned}$$

Thus, we have $d \in D^1_+$, and the corresponding 1-cocycle is c. □

Remark 8.7. It follows from the injectivity of (8.3) that the right hand side of (8.11) does not depend on the choice of the lift of $\vartheta(c) \in \mathbb{A}^r \otimes_{\mathbb{Z}[F]} \mathrm{Lie}(\mathbb{A})$ to $\mathbb{A}^r \otimes \mathrm{Lie}(\mathbb{A})$. This can also be checked directly using (A.27) and Lemma 5.6.

9. The Lie algebra of oriented trees with beads

In this section, we define the Lie algebra of oriented trees with beads, and give a diagrammatic description of the Lie algebra of special derivations $D^0_+ \simeq \mathrm{Der}^\zeta_+(\overline{\mathsf{A}}_\bullet) \simeq D^1_+$ with rational coefficients.

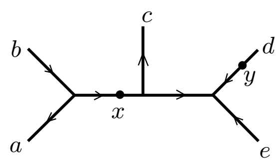
9.1. **Trees with beads.** We start with a general study of certain spaces of "trees", which are "tree-shaped Jacobi diagrams with beads", see Remark 9.2.

By a *tree* we mean a finite simply-connected graph with only univalent vertices (called *leaves*) and trivalent vertices (called *nodes*). A tree is *edge-oriented* if each edge is oriented, *node-oriented* if a cyclic order of the three edges incident at each vertex is specified, and *oriented* if it is both edge-oriented and node-oriented. In figures, the edge-orientations are shown with little arrows, and we agree that node-orientations are always given by the counter-clockwise direction.

Let V and H be sets. A tree T is said to be *on* V if all its leaves are colored by elements of V, and it is said to have *H-beads* if some of its edges are colored by elements of H. In figures, the edges that are colored by H are decorated with beads.

We define the *degree* of a tree T to be 1 plus the number of nodes of T, which equals the number of leaves of T minus 1.

Example 9.1. Here is an oriented tree on V with H-beads of degree 4:



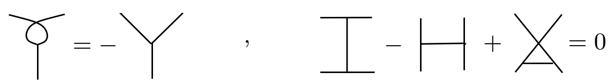
(with $a, b, c, d, e \in V$, $x, y \in H$)

In the following, let $H = (H, \Delta, \varepsilon, S)$ be a cocommutative Hopf $\mathbb{Q}$-algebra and V a left H-module. Consider the $\mathbb{Q}$-vector space

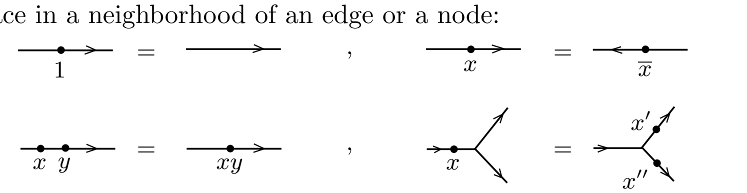
$$\mathcal{D}(V, H) := \frac{\mathbb{Q} \cdot \{\text{oriented trees on } V \text{ with } H\text{-beads}\}}{\text{AS, IHX, multilinearity, Hopf, bead-out}}$$

where the relations are defined as follows.

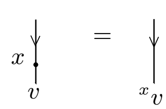
- The *AS* and *IHX* relations take place in a neighborhood of a node and an internal edge, respectively:



  (No beads should appear here, and the edge-orientations are arbitrary).
- The *multilinearity* relations require $\mathbb{Q}$-multilinearity for the colors at the leaves and edges.
- The *Hopf* relations involve the Hopf algebra structure of H, and they take place in a neighborhood of an edge or a node:



  (Here the antipode $S(x)$ of an $x \in H$ is denoted by $\overline{x}$ and the coproduct $\Delta(x) = x' \otimes x''$ is expanded using Sweedler's notation.)
- The *bead-out* relation takes place in a neighborhood of a leaf, and it involves the H-action on V:



We obtain a graded $\mathbb{Q}$-vector space

$$\mathcal{D}(V, H) = \bigoplus_{k=1}^{\infty} \mathcal{D}_k(V, H)$$

where the degree k part of $\mathcal{D}(V, H)$ is spanned by the trees of degree k.

Remark 9.2. Oriented trees with beads are an instance of "Jacobi diagrams with beads", which appear in the theory of finite-type invariants, see e.g. [GL01], [HM21].

We will define a $\mathbb{Q}$-vector space $\mathcal{K}(V,H)$, which is isomorphic to $\mathcal{D}(V,H)$ by Proposition 9.4 below. The (left) H-action on V extends to that on $\mathrm{Lie}(V)$, the free Lie algebra on V, by the inductive rule

$$x \cdot [u,v] = [x' \cdot u, x'' \cdot v] \quad (x \in H,\ u,v \in \mathrm{Lie}(V)).$$

Let V^r denote V with the right H-action defined by $v^h := {}^{\overline{h}}v$ ($v \in V,\ h \in H$). Since the Lie bracket $[-,-] : V \otimes_{\mathbb{Q}} \mathrm{Lie}(V) \to \mathrm{Lie}(V)$ is a H-module map, it induces a $\mathbb{Q}$-linear map

$$\beta : V^r \otimes_H \mathrm{Lie}(V) \simeq \big(V \otimes_{\mathbb{Q}} \mathrm{Lie}(V)\big)_H \longrightarrow \mathrm{Lie}(V)_H$$

where $W_H = W/\big(\ker(\varepsilon)\cdot W\big)$ denotes the space of H-coinvariants of W for any H-module W. Then, we define the $\mathbb{Q}$-vector space

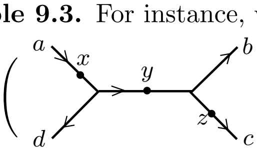
$$\mathcal{K}(V,H) := \ker(\beta) \ \subset\ V^r \otimes_H \mathrm{Lie}(V),$$

which is graded with degree k part $\mathcal{K}_k(V,H) = \mathcal{K}(V,H) \cap (V^r \otimes_H \mathrm{Lie}_k(V))$.

Let D be a tree in $\mathcal{D}(V,H)$ of degree k, and ℓ a leaf of D. Let $\mathrm{col}(\ell) \in V$ denote the color of ℓ. We reorient the tree T (if necessary) by using the second Hopf relation to have all edges of T oriented *outwards* ℓ, and we then let $\mathrm{word}(\ell) \in \mathrm{Lie}_k(V)$ denote the Lie word that is encoded by the tree D rooted at ℓ, where each bead colored by an $x \in H$ is interpreted as a (left) action of x on the outer subtree. Then set

$$\eta(D) := \sum_{\ell:\mathrm{leaf}} \mathrm{col}(\ell) \otimes \mathrm{word}(\ell) \ \in V^r \otimes_H \mathrm{Lie}_k(V). \tag{9.1}$$

Example 9.3. For instance, we have

$\eta\Big($  $\Big)$

$$= a \otimes {}^{x}\big[{}^{y}[b, {}^{z}c], d\big] + b \otimes \big[{}^{z}c, {}^{\overline{y}}[d, {}^{\overline{x}}a]\big]$$
$$+ c \otimes {}^{\overline{z}}\big[{}^{\overline{y}}[d, {}^{\overline{x}}a], b\big] + d \otimes \big[{}^{\overline{x}}a, {}^{y}[b, {}^{z}c]\big].$$

Proposition 9.4. *Assume that* $\mathrm{Tor}_1^H\big(\ker(\varepsilon), \mathrm{Lie}(V)\big) = 0$. *Then* (9.1) *defines an isomorphism* $\eta : \mathcal{D}(V,H) \to \mathcal{K}(V,H)$ *of graded* $\mathbb{Q}$*-vector spaces.*

Remark 9.5. The $\mathbb{Q}$-vector space $\mathrm{Tor}_1^H\big(\ker(\varepsilon), \mathrm{Lie}(V)\big) \simeq H_2\big(H; \mathrm{Lie}(V)\big)$ vanishes if V is a projective H-module or if we have $H = \mathbb{Q}[F]$ with F a free group.

Proof of Proposition 9.4. Consider the following graded $\mathbb{Q}$-vector space, which depends only on V:

$$\mathcal{D}(V) := \frac{\mathbb{Q}\cdot\{\text{node-oriented trees on } V\}}{\text{AS, IHX, multilinearity}}.$$

Every generator D of $\mathcal{D}(V)$ of degree k is transformed to an element $\eta(D) \in V \otimes_{\mathbb{Q}} \mathrm{Lie}_k(V)$ using the same formula as (9.1). It is well known that one defines in this way a $\mathbb{Q}$-linear isomorphism

$$\eta : \mathcal{D}(V) \longrightarrow \mathcal{K}(V) \quad \text{where } \mathcal{K}(V) := \ker\big([-,-] : V \otimes_{\mathbb{Q}} \mathrm{Lie}(V) \to \mathrm{Lie}(V)\big), \tag{9.2}$$

see e.g. [HP03].

The (left) action of H on V extends to that on $\mathcal{D}(V)$ using the coproduct of H. Consider the space of H-coinvariants

$$\mathcal{D}(V)_H = \mathcal{D}(V)\,/\,\ker(\varepsilon)\cdot\mathcal{D}(V). \tag{9.3}$$

Since (9.2) is a H-module isomorphism, it induces a linear isomorphism $\eta_H : \mathcal{D}(V)_H \to \mathcal{K}(V)_H$. By the snake lemma we easily see that the kernel of the canonical map $\mathcal{K}(V) \to \mathcal{K}(V,H)$ is the kernel of

$$\ker(\varepsilon) \otimes_H [-,-] : \ker(\varepsilon) \cdot \big(V \otimes_{\mathbb{Q}} \mathrm{Lie}(V)\big) \longrightarrow \ker(\varepsilon) \cdot \mathrm{Lie}(V)$$

and, by the flatness assumption, this is $\ker(\varepsilon)\cdot\mathcal{K}(V)$. Therefore, we have a canonical isomorphism $\mathcal{K}(V)_H \simeq \mathcal{K}(V,H)$, so that we can view η_H as an isomorphism between $\mathcal{D}(V)_H$ and $\mathcal{K}(V,H)$.

We have a natural $\mathbb{Q}$-linear map $\mathcal{D}(V) \to \mathcal{D}(V,H)$. The Hopf and bead-out relations in $\mathcal{D}(V,H)$ imply that this map is surjective and vanishes on $\ker(\varepsilon)\cdot\mathcal{D}(V)$. Therefore, it induces a surjective $\mathbb{Q}$-linear map $u : \mathcal{D}(V)_H \to \mathcal{D}(V,H)$.

It is easily checked that (9.1) defines a map $\eta : \mathcal{D}(V,H) \to V^r \otimes_H \mathrm{Lie}(V)$, and, clearly, we have $\eta \circ u = \eta_H$. Since u is surjective and η_H is an isomorphism, we conclude that η is an isomorphism onto the subspace $\mathcal{K}(V,H)$ of $V^r \otimes_H \mathrm{Lie}(V)$. □

9.2. **Diagrammatic description of $D_+^0 \simeq D_+^1$ with rational coefficients.** We now restrict to the case where $H := \mathbb{Q}[F]$ and $V := \mathbb{A}^{\mathbb{Q}} = \mathbb{A} \otimes \mathbb{Q}$. Thus, we consider the space

$$\mathcal{D} := \mathcal{D}(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$$

of trees on $\mathbb{A}^{\mathbb{Q}}$ with $\mathbb{Q}[F]$-beads. Note that $\mathcal{K}(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$ is isomorphic to $D_+^0 \otimes \mathbb{Q}$ via the identification ϑ^{-1} of Lemma 8.1. Hence, by Proposition 9.4, we get an isomorphism of graded $\mathbb{Q}$-vector spaces

$$\eta : \mathcal{D} \xrightarrow{\simeq} D_+^0 \otimes \mathbb{Q}. \tag{9.4}$$

The following describes the derivation of $\mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ corresponding to an element of $\mathcal{D}$.

Proposition 9.6. *Let D be a tree on $\mathbb{A}^{\mathbb{Q}}$ with $\mathbb{Q}[F]$-beads, and let $d \in D_+^1 \otimes \mathbb{Q}$ be the derivation corresponding to $\eta(D) \in D_+^0 \otimes \mathbb{Q}$. Then, for any $a \in \mathbb{A}^{\mathbb{Q}}$, we have*

$$\begin{aligned} d(a) \quad = \quad & -\sum_v \Big[\overline{\Psi(\mathrm{col}(v),a)^\ell} \cdot \mathrm{word}(v), \Psi(\mathrm{col}(v),a)^r\Big] \\ & + \sum_b \overline{\langle \mathrm{col}(b)', a\rangle} \cdot \Big[\mathrm{word}^\ell(b), \mathrm{col}(b)'' \cdot \mathrm{word}^r(b)\Big]. \end{aligned} \tag{9.5}$$

Here the first sum is over all leaves v of D and uses the same notations as (9.1), and the second sum is over all beads b of D. The element $\mathrm{col}(b) \in \mathbb{Q}[F]$ is the color of b, while the elements $\mathrm{word}^\ell(b), \mathrm{word}^r(b) \in \mathrm{Lie}(V)$ are represented by the two half-trees obtained by cutting D at b (orienting all the edges of these half-trees outwards b, deleting the bead b from both, and assuming that $\mathrm{word}^\ell(b)$ comes before $\mathrm{word}^r(b)$ if one follows the original orientation of the edge around b).

Proof. If D has no bead, then (9.5) immediately follows from (9.1) and (8.11). Since the $\mathbb{Q}$-vector space $\mathcal{D}$ is generated by trees without bead, it suffices to show that (for a fixed) the right-hand side of (9.5) defines a $\mathbb{Q}$-linear form on $\mathcal{D}$. To prove this, we need to check that each defining relation of $\mathcal{D}$ is mapped to 0. This consists in straightforward verification whose key arguments are given in Table 2. □

The Lie bracket on $D_+^0 \otimes \mathbb{Q}$ transports through η to a Lie bracket on $\mathcal{D}$. We now aim at giving an explicit description of this Lie bracket $[D,E]$ for any two trees

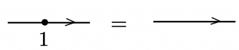
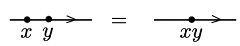
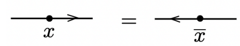
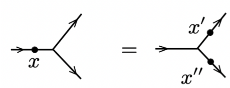
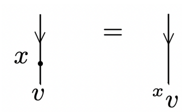
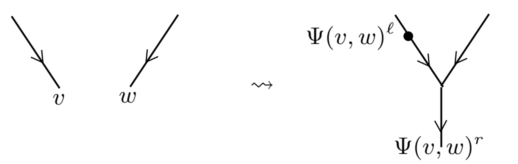
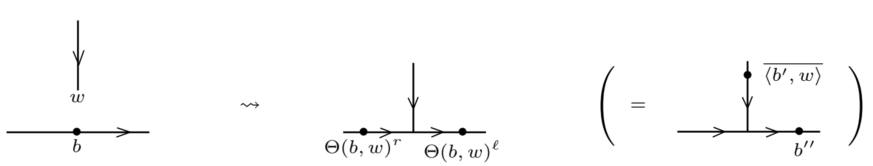
Defining relation of $\mathcal{D}$	**Argument**
multilinearity	$\mathbb{Q}$-bilinearity of Ψ and $\langle -, - \rangle$
	Property (A.2)
	Property (A.2)
	Property (A.2)
	Axioms of Lie($\mathbb{A}$)
IHX	Axioms of Lie($\mathbb{A}$)
AS	Axioms of Lie($\mathbb{A}$)
	Property(A.27) & formula (A.21)

TABLE 2.

D, E in $\mathcal{D}$. For any leaves v and w of D and E, respectively, let $D \overset{v,w}{\vee} E$ be the $\mathbb{Q}$-linear combination of trees defined by "branching" as follows:



Here we use the rationalization $\Psi : \mathbb{A}^{\mathbb{Q}} \times \mathbb{A}^{\mathbb{Q}} \to \mathbb{Q}[F] \otimes_{\mathbb{Q}} \mathbb{A}^{\mathbb{Q}}$ of the intersection operation (A.25), and we have omitted the symbols $\mathrm{col}(-)$ on the right-hand side for simplicity. Similarly, for any bead b of D and for any leaf w of E, let $D \overset{b,w}{\perp} E$ be the $\mathbb{Q}$-linear combination of trees defined by "grafting" as follows:



Here we use the rationalization $\Theta : \mathbb{Q}[F] \times \mathbb{A}^{\mathbb{Q}} \to \mathbb{Q}[F] \otimes_{\mathbb{Q}} \mathbb{Q}[F]$ of the intersection operation (A.20), and the indicated identity follows from (A.21).

Theorem 9.7. *Let D, E be oriented trees on $\mathbb{A}^{\mathbb{Q}}$ with $\mathbb{Q}[F]$-beads. Then we have*

$$[D, E] = \sum_{v,w} D \overset{v,w}{\vee} E - \sum_{b,w} D \overset{b,w}{\perp} E + \sum_{v,c} E \overset{c,v}{\perp} D \ \in \mathcal{D}, \tag{9.6}$$

where v (resp. w) runs over all leaves of D (resp. E), and b (resp. c) runs over all beads of D (resp. E).

Proof. We claim that the right-hand side of (9.6) defines a binary operation in the space $\mathcal{D}$. To prove this, we need to verify that each defining relation of $\mathcal{D}$ is mapped to 0. This is a straightforward verification, which is left to the reader. Table 3 gives the key arguments that are involved for each of those relations.

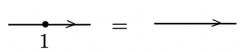
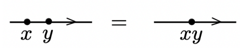
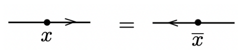
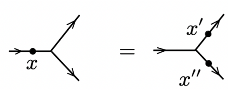
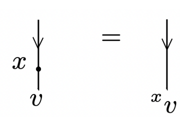
Defining relation of $\mathcal{D}$	**Argument**
multilinearity	$\mathbb{Q}$-bilinearity of Θ and Ψ
	Property (A.22)
	Property (A.22)
	Property (A.24)
	IHX
IHX	IHX
AS	AS
	Properties (A.23), (A.27) & (A.28)

TABLE 3.

We now aim at proving that the Lie bracket $[D, E]$ is equal to the right-hand side of (9.6). Since the $\mathbb{Q}$-vector space $\mathcal{D}$ is generated by trees without bead, we can assume that D and E have no bead. Set $c := \eta(D)$ and $g := \eta(E)$, and let $d, e \in D_+^1 \otimes \mathbb{Q}$ be the derivations corresponding to $c, g \in D_+^0 \otimes \mathbb{Q}$, respectively. Then, by Proposition 9.6, we have

$$d(a) = -\sum_v \left[\overline{\Psi(v,a)^\ell} \cdot \mathrm{word}(v), \Psi(v,a)^r\right] \quad \text{for all } a \in \mathbb{A}^{\mathbb{Q}},$$

where the sum is over all leaves v of D and we have denoted $\mathrm{col}(v)$ simply by v. Therefore, for any $a \in \mathbb{A}^{\mathbb{Q}}$, we get $e(d(a)) = L(a) + M(a) + N(a)$ with

$$\begin{aligned} L(a) \quad &:= \quad -\sum_v \left[\overline{\Psi(v,a)^\ell} \cdot e(\mathrm{word}(v)), \Psi(v,a)^r\right] \\ M(a) \quad &:= \quad -\sum_v \left[\left[g\big((\overline{\Psi(v,a)^\ell})'\big), \big(\overline{\Psi(v,a)^\ell}\big)'' \cdot \mathrm{word}(v)\right], \Psi(v,a)^r\right] \\ &= \quad \sum_v \left[\overline{\Psi(v,a)^{\ell'}} \cdot \left[g\big(\Psi(v,a)^{\ell''}\big), \mathrm{word}(v)\right], \Psi(v,a)^r\right] \end{aligned}$$

$$N(a) \quad := \quad -\sum_{v} \left[\overline{\Psi(v,a)^{\ell}} \cdot \mathrm{word}(v), e\big(\Psi(v,a)^{r}\big)\right],$$

where, in the sum $M(a)$, we have used Sweedler's notation for the coproduct of $\overline{\Psi(v,a)^{\ell}}$. We get a similar formula $d(e(a)) = P(a) + Q(a) + R(a)$ by exchanging the roles of D and E. It follows from the above computation that the Lie bracket $[d,e]$ of the derivations d,e maps any $a \in \mathbb{A}^{\mathbb{Q}}$ to

$$d(e(a)) - e(d(a)) = P(a) + Q(a) + R(a) - L(a) - M(a) - N(a). \tag{9.7}$$

Since D and E have no bead, the right-hand side of (9.6) reduces to the sum $\sum_{v,w} D \overset{v,w}{\vee} E$. Besides, according to Proposition 9.6, the derivation in $D_{+}^{1} \otimes \mathbb{Q}$ corresponding to $\eta\big(\sum_{v,w} D \overset{v,w}{\vee} E\big)$ maps an $a \in \mathbb{A}^{\mathbb{Q}}$ to $\big(X(a)+Y(a)+Z(a)\big)+W(a)$, where

$$\begin{aligned}
X(a) &= -\sum_{v,w} \left[\overline{\Psi\big(\Psi(v,w)^{r},a\big)^{\ell}} \cdot [\overline{\Psi(v,w)^{\ell}} \cdot \mathrm{word}(v), \mathrm{word}(w)], \Psi\big(\Psi(v,w)^{r},a\big)^{r}\right],\\
Y(a) &= -\sum_{v,w,v'\neq v} \left[\overline{\Psi(v',a)^{\ell}} \cdot \big(\mathrm{word}(v')\big|_{v\mapsto \Psi(v,w)^{\ell}\cdot[\mathrm{word}(w),\Psi(v,w)^{r}]}\big), \Psi(v',a)^{r}\right],\\
Z(a) &= -\sum_{v,w,w'\neq w} \left[\overline{\Psi(w',a)^{\ell}} \cdot \big(\mathrm{word}(w')\big|_{w\mapsto [\Psi(v,w)^{r},\overline{\Psi(v,w)^{\ell}}\cdot \mathrm{word}(v)]}\big), \Psi(w',a)^{r}\right],\\
W(a) &= \sum_{v,w} \overline{\langle \Psi(v,w)^{\ell'}, a\rangle} \cdot \left[\mathrm{word}(v), \Psi(v,w)^{\ell''} \cdot [\mathrm{word}(w), \Psi(v,w)^{r}]\right].
\end{aligned}$$

In the sum $Y(a)$, the third index runs over all leaves v' of D different from v, and the notation $\mathrm{word}(v')|_{v\mapsto u}$ means that $\mathrm{word}(v') \in \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ is transformed into another word by inserting $u \in \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ in place of the letter v; a similar remark applies to the sum $Z(a)$. It is easily seen that $Z(a) = P(a)$ and, using (A.29), that $Y(a) = -L(a)$. Therefore, by comparison with (9.7), it suffices to prove the following identity:

$$Q(a) + R(a) - M(a) - N(a) = X(a) + W(a). \tag{9.8}$$

To prove this, we come back to $M(a) + N(a)$ and we simplify our notations further by denoting, for any leaf v, the corresponding element $\mathrm{word}(v)$ of $\mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ by the corresponding upper-case letter V:

$$\begin{aligned}
&M(a) + N(a)\\
=\ & \sum_{v,w} \left[\overline{\Psi(v,a)^{\ell'}} \cdot \left[\big\langle \Psi(v,a)^{\ell''}, w\big\rangle \cdot W, V\right], \Psi(v,a)^{r}\right]\\
&+ \sum_{v,w} \left[\overline{\Psi(v,a)^{\ell}} \cdot V, \left[\overline{\Psi(w,\Psi(v,a)^{r})^{\ell}} \cdot W, \Psi(w,\Psi(v,a)^{r})^{r}\right]\right]\\
=\ & -\sum_{v,w} \left[\overline{\Psi(v,a)^{\ell'''}} \cdot V, \left[\left(\overline{\Psi(v,a)^{\ell'}}\big\langle \Psi(v,a)^{\ell''}, w\big\rangle\right) \cdot W, \Psi(v,a)^{r}\right]\right]\\
&+ \sum_{v,w} \left[\left(\overline{\Psi(v,a)^{\ell'}}\big\langle \Psi(v,a)^{\ell''}, w\big\rangle\right) \cdot W, \left[\overline{\Psi(v,a)^{\ell'''}} \cdot V, \Psi(v,a)^{r}\right]\right]\\
&+ \sum_{v,w} \left[\overline{\Psi(v,a)^{\ell}} \cdot V, \left[\overline{\Psi(w,\Psi(v,a)^{r})^{\ell}} \cdot W, \Psi(w,\Psi(v,a)^{r})^{r}\right]\right].
\end{aligned}$$

Therefore, a symmetric computation for $Q(a)+R(a)$ gives

$$\begin{aligned} & M(a)+N(a)-Q(a)-R(a) \\ = & \Bigg(-\sum_{v,w} \Big[\overline{\Psi(v,a)^{\ell'''}}\cdot V, \Big[\Big(\overline{\Psi(v,a)^{\ell'}}\langle \Psi(v,a)^{\ell''}, w\rangle\Big)\cdot W, \Psi(v,a)^r\Big]\Big] \\ & +\sum_{v,w} \Big[\overline{\Psi(v,a)^{\ell}}\cdot V, \Big[\overline{\Psi(w,\Psi(v,a)^r)^{\ell}}\cdot W, \Psi(w,\Psi(v,a)^r)^r\Big]\Big] \\ & -\sum_{w,v} \Big[\Big(\overline{\Psi(w,a)^{\ell'}}\langle \Psi(w,a)^{\ell''}, v\rangle\Big)\cdot V, \Big[\overline{\Psi(w,a)^{\ell'''}}\cdot W, \Psi(w,a)^r\Big]\Big]\Bigg) \\ & -\big(\text{the symmetric counterpart } D\leftrightarrow E\big). \end{aligned}$$

Next, a double application of (A.31) leads to

$$\begin{aligned} & M(a)+N(a)-Q(a)-R(a) \\ = & \sum_{v,w} \Big[\overline{\Psi(\Psi(w,v)^r,a)^{\ell'}}\cdot V, \Big[\overline{\Psi(w,v)^{\ell}\,\Psi(\Psi(w,v)^r,a)^{\ell''}}\cdot W, \Psi(\Psi(w,v)^r,a)^r\Big]\Big] \\ & -\sum_{w,v} \Big[\overline{\Psi(\Psi(v,w)^r,a)^{\ell'}}\cdot W, \Big[\overline{\Psi(v,w)^{\ell}\,\Psi(\Psi(v,w)^r,a)^{\ell''}}\cdot V, \Psi(\Psi(v,w)^r,a)^r\Big]\Big]. \end{aligned}$$

Here, the first sum can be transformed by applying (A.29) to $\Psi(w,v)$ and by using (A.27) next, which results in the following identity:

$$\begin{aligned} & M(a)+N(a)-Q(a)-R(a) \\ = & -\sum_{v,w} \Bigg[\overline{\Theta(\Psi(v,w)^{\ell''},a)^{r'}}\cdot V, \\ & \qquad \Big[\Big(\overline{\Theta(\Psi(v,w)^{\ell''},a)^{r''}\,\Psi(v,w)^{\ell'}}\Big)\cdot W, \Theta(\Psi(v,w)^{\ell''},a)^{\ell}\cdot \Psi(v,w)^r\Big]\Bigg] \\ & +\sum_{v,w} \Big[\overline{\Psi(v,w)^{\ell}\,\Psi(\Psi(v,w)^r,a)^{\ell'}}\cdot V, \Big[\overline{\Psi(\Psi(v,w)^r,a)^{\ell''}}\cdot W, \Psi(\Psi(v,w)^r,a)^r\Big]\Big] \\ & -\sum_{w,v} \Big[\overline{\Psi(\Psi(v,w)^r,a)^{\ell'}}\cdot W, \Big[\overline{\Psi(v,w)^{\ell}\,\Psi(\Psi(v,w)^r,a)^{\ell''}}\cdot V, \Psi(\Psi(v,w)^r,a)^r\Big]\Big]. \end{aligned}$$

In this last identity, the first term can be seen to coincide with $-W(a)$, while the second and third terms give $-X(a)$. This proves (9.8). $\square$

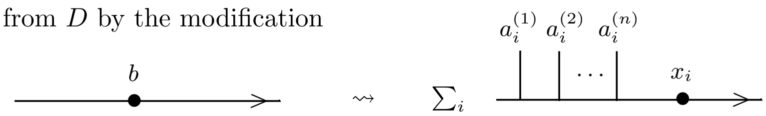
Remark 9.8. We can directly prove that the binary operation (9.6) in $\mathcal{D}$ satisfies the axioms of a Lie bracket. Since the space $\mathcal{D}$ is generated by trees without beads, it is enough to verify the antisymmetry $[D,E]=-[E,D]$ and the Jacobi identity $[[D,E],F]+[[F,D],E]+[[E,F],D]=0$ for trees D,E,F with no bead. Then, the antisymmetry is easily deduced from (A.29), and the Jacobi identity can be proved by a long computation using (A.30) and (A.31). Note that, in the proof of Proposition A.5, the latter identities are derived from (A.11), which is a form of "quasi-Jacobi" identity satisfied by the intersection double bracket [MT14].

The space $\mathcal{D}=\mathcal{D}(\mathbb{A}^{\mathbb{Q}},\mathbb{Q}[F])$ has another description, which will be used in the next section in a few places. Consider the space

$$\mathcal{D}' := \mathcal{D}\big(\mathrm{Lie}(\mathbb{A}^{\mathbb{Q}}), T(\mathbb{A}^{\mathbb{Q}})\otimes_{\mathbb{Q}}\mathbb{Q}[F]\big)$$

of trees on $\mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ with $\big(T(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]\big)$-beads. Here $T(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$ is viewed as the universal enveloping algebra of the extended graded Lie algebra $\overline{\mathsf{A}}^{\mathbb{Q}}_{\bullet}$. The adjoint action of this cocommutative Hopf algebra on itself restricts to an action on $\mathrm{Lie}(\mathbb{A}^{\mathbb{Q}}) = \overline{\mathsf{A}}^{\mathbb{Q}}_{+}$. We consider the following two types of operations on an arbitrary tree $D \in \mathcal{D}'$:

- The *expansion* of D at a leaf ℓ is the element $D_\ell \in \mathcal{D}'$ that is obtained from D by representing $\mathrm{col}(\ell) \in \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ as a linear combination of half-trees with $\mathbb{A}^{\mathbb{Q}}$-colored leaves. (That D_ℓ is well-defined follows from the AS, IHX and multilinearity relations.)
- The *expansion* of D at a bead b is the element $D_b \in \mathcal{D}'$ that is obtained from D by the modification



  if b is colored by $\sum_i a_i^{(1)} \cdots a_i^{(n_i)} x_i$ with $a_i^{(1)}, \dots, a_i^{(n_i)} \in \mathbb{A}^{\mathbb{Q}}$ and $x_i \in \mathbb{Q}[F]$. (That D_b is well-defined follows from the multilinearity relations.)

Let $\mathcal{E}$ be the subspace of $\mathcal{D}'$ generated by the differences $D - D_\ell$ and $D - D_b$, for all trees $D \in \mathcal{D}'$, leaf ℓ of D and bead b of D. (In fact, it is easily checked from the "bead-out" relation that the expansions of beads follow from expansions of leaves.)

Lemma 9.9. *The $\mathbb{Q}$-linear map $f : \mathcal{D} \to \mathcal{D}'/\mathcal{E}$ that is induced by the inclusions $\mathbb{A}^{\mathbb{Q}} \subset \mathrm{Lie}(\mathbb{A}^{\mathbb{Q}})$ and $\mathbb{Q}[F] \subset T(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$ is an isomorphism.*

Proof. Clearly, f is surjective. For any tree $D \in \mathcal{D}'$, let $e(D) \in \mathcal{D}$ be obtained from D by expanding all its leaves and all its beads at the same time. It is easily checked that the assignment $D \mapsto e(D)$ defines a $\mathbb{Q}$-linear map $e : \mathcal{D}'/\mathcal{E} \to \mathcal{D}$. Clearly, $e \circ f$ is the identity. □

10. Some formulas and examples

In this section, we provide some explicit formulas for Johnson homomorphisms, which are based on the diagrammatic descriptions of Section 9. As an example, we also consider the restriction of the Johnson filtration to the pure braid group.

10.1. **The first Johnson homomorphism on disk twists.** The next proposition computes the first Johnson homomorphism on a disk twist.

Proposition 10.1. *For any properly embedded disk $U \subset V$, we have*

$$\tau_1^0(T_{\partial U}) = -\eta\Big(\frac{1}{2}[u] — [u]\Big) \in Z^1(F, \mathbb{A}), \tag{10.1}$$

where $u \in \mathsf{A}$ is the homotopy class of the closed curve ∂U (with an arbitrary orientation, and an arbitrary basing at $\star$) and $[u] \in \mathbb{A}$ is the corresponding class.

Proof. Note that, as a consequence of the bead-out relation, the right-hand side of (10.1) does not depend on the choice of $u \in \mathsf{A}$. Let U' be a closed curve in Σ which is isotopic to ∂U and satisfies $U' \cap \partial\Sigma = \{\star\}$. Hence, by orienting U' arbitrarily and by regarding it as a loop based at $\star$, we can take $u := [U'] \in \mathsf{A}$.

We shall use the same notation as in §A.1. In particular, let $\bullet$ be a second base-point in $\partial\Sigma$. Let $x \in \pi$ and let X be a loop based at $\bullet$ such that $(\overline{\partial\Sigma})_{\star\bullet}\, X\, (\partial\Sigma)_{\bullet\star}$ represents x. We assume that X meets U' transversely in finitely many double points, which are numbered $1, \dots, n$, and appear in this order along X. Then we have

$$(T_{\partial U}(x))\, x^{-1} = \Big[\prod_{i=1}^{n} (\overline{\partial \Sigma})_{\star \bullet}\, X_{\bullet i}\, (U')_i^{\varepsilon_i}\, \overline{X}_{i \bullet}\, (\partial \Sigma)_{\bullet \star}\Big] \in \pi,$$

where $\varepsilon_i = \varepsilon_i(U', X) \in \{-1, +1\}$ is the sign of the intersection of U' and X at i, and $(U')_i^{\varepsilon_i}$ denotes the loop U' based at i, with the opposite orientation if $\varepsilon_i = -1$. Hence the 1-cocycle $\tau_1^0(T_{\partial U})$ maps $[x] \in F$ to

$$\sum_{i=1}^{n} \varepsilon_i \left[(\overline{\partial \Sigma})_{\star \bullet}\, X_{\bullet i}\, U'_i\, \overline{X}_{i \bullet}\, (\partial \Sigma)_{\bullet \star}\right] \in \mathbb{A}. \tag{10.2}$$

Besides, using now the notations of §A.3, we have

$$\langle [x], [u] \rangle \;=\; \varpi\big(\eta(x, u)\big) \;=\; -\sum_{i=1}^{n} \varepsilon_i \left[(\overline{\partial \Sigma})_{\star \bullet} X_{\bullet i} U'_{i \star}\right] \in \mathbb{Z}[F].$$

Thus, the action of $-\langle [x], [u] \rangle$ on $[u]$ gives (10.2), which completes the proof of (10.1). □

Remark 10.2. Recall from Example 7.1 that $\tau_1^0 : \mathcal{T} \to Z^1(F, \mathbb{A})$ is equivalent to the Magnus representation $\mathrm{Mag} = \mathrm{Mag}_1^0 : \mathcal{T} \to \mathrm{Mat}(g \times g; \mathbb{Z}[F])$. Tracing the sequence of isomorphisms (4.9) and taking into account Proposition 6.2, it is easily checked that, for any $f \in \mathcal{T}$ with Magnus representation $M = (m_{ij})_{i,j}$,

$$\eta^{-1}\big(\tau_1^0(f)\big) = -\frac{1}{2} \sum_{i,j=1}^{g} a_i \overset{m_{ij}}{-\!\!\bullet\!\!\!\longrightarrow\!\!-} a_j. \tag{10.3}$$

For instance, for the Dehn twist along the boundary curve, Proposition 10.1 gives

$$\eta^{-1}\big(\tau_1^0(T_{\partial \Sigma})\big) = -\frac{1}{2}[\zeta]\!-\!\!-\![\zeta] \overset{(6.2)}{=} -\frac{1}{2} \sum_{i,j=1}^{g} \big((1 - x_i^{-1}) \cdot a_i\big)\!-\!\!-\!\!-\!\big((1 - x_j^{-1}) \cdot a_j\big)$$

and we recover our previous computation (6.10) of $\mathrm{Mag}(T_{\partial \Sigma})$.

Proposition 10.1 gives a new proof of a result of McCullough [Mc84, Th. 1.2].

Theorem 10.3 (McCullough). *If $g \geq 2$, then the twist group $\mathcal{T}$ surjects onto a free abelian group of countably-infinite rank. In particular, $\mathcal{T}$ is not finitely generated.*

Proof. Let $p : \mathbb{Z}[F] \to \mathbb{Z}[\mathbb{Z}]$ be the ring homomorphism induced by the homomorphism $F \to \mathbb{Z}$ that maps every x_i to 1. By reducing coefficients with p, the Magnus representation induces a homomorphism $\mathrm{Mag}^p : \mathcal{T} \to \mathrm{Mat}(g \times g; \mathbb{Z}[t^{\pm 1}])$.

The upper-left corner of Mag^p provides a homomorphism $m : \mathcal{T} \to \mathbb{Z}[t^{\pm 1}]$. By Proposition 6.2, m takes values in the subgroup S of $\mathbb{Z}[t^{\pm 1}]$ generated by 1 and $t^n + t^{-n}$ for all $n \in \mathbb{Z}$. It suffices to prove $m(\mathcal{T}) = S$.

For any $n \in \mathbb{Z}$, there is a simple closed curve γ_n in Σ, whose homotopy class (for an appropriate orientation and basing at $\star$) is of the form

$$\alpha'_1 z_n \alpha_1^{-1} z_n^{-1} \in \mathsf{A} \subset \pi,$$

where α_1, α'_1 are the loops shown in (7.5), and $z_n \in \pi$ satisfies $\varpi(z_n) = x_2^n \in F$. By Proposition 10.1, we have

$$\eta^{-1}\tau_1^0(T_{\gamma_n}) = -\frac{1}{2}(x_1^{-1} \cdot a_1 - x_2^n \cdot a_1)\!-\!\!-\!(x_1^{-1} \cdot a_1 - x_2^n \cdot a_1),$$

and we deduce from (10.3) that

$$m(T_{\gamma_n}) = (t - t^{-n})(t^{-1} - t^n) = 2 - t^{n+1} - t^{-n-1}.$$

Besides, by considering now the curve α_1, we obtain

$$\eta^{-1}\tau_1^0(T_{\alpha_1}) = -\frac{1}{2}a_1 \text{—} a_1, \quad \text{hence } m(T_{\alpha_1}) = 1.$$

Thus, products of Dehn twists (and their inverses) along the curves α_1 and γ_n (for $n \in \mathbb{Z}$) realize any element of S. □

Remark 10.4. Some arguments similar to the proof of Theorem 10.3 show that $\mathrm{Mag}^p : \mathcal{T} \to \mathrm{Mat}\big(g \times g; \mathbb{Z}[t^{\pm 1}]\big)$ is surjective onto the subgroup of hermitian matrices, for $g \geq 3$. In fact, the above proof is inspired by the arguments in [Mc84], which involve an infinite-cyclic cover of the handlebody V.

10.2. **An analogue of the Kawazumi–Kuno formula.** Proposition 10.1 is fully generalized by the following result, where the isomorphism of Lemma 9.9 is implicit.

Theorem 10.5. *For any special expansion θ of the free pair $(\pi, \mathbb{A})$ and for any properly embedded disk $U \subset V$, we have*

$$\varrho^\theta(T_{\partial U}) = -\eta\Big(\frac{1}{2}\log\theta(u) \text{—} \log\theta(u)\Big), \tag{10.4}$$

where $u \in \mathsf{A}$ is the homotopy class of the closed curve ∂U (with an arbitrary orientation and basing at $\star$).

The proof involves the Kawazumi–Kuno formula for the logarithms of Dehn twists [KK14]. To derive (10.4) from the Kawazumi–Kuno formula, we first need to relate precisely the notion of "special expansion" for the free pair (π, A) to the notion of "symplectic expansion" for the free group π. Recall from [Mas12] that an *expansion* of the free group π is a monoid homomorphism $\tilde\theta : \pi \to \widehat{T}(H^{\mathbb{Q}})$, with values in the degree-completed tensor algebra on $H^{\mathbb{Q}} := H_1(\pi; \mathbb{Q})$, such that $\tilde\theta(x)$ is group-like for every $x \in \pi$ and satisfies $\log\tilde\theta(x) = [x] + (\deg \geq 2)$. Furthermore, the expansion $\tilde\theta$ is said to be *symplectic* if

$$\tilde\theta(\zeta) = \exp([\zeta]_2), \tag{10.5}$$

where $[\zeta]_2 \in \Gamma_2\pi/\Gamma_3\pi \simeq \Lambda^2 H^{\mathbb{Q}}$ is regarded as a tensor of degree 2.

Lemma 10.6. *There exists a special expansion $\theta : \pi \to \hat{T}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$ of (π, A) and an injective $\mathbb{Q}$-algebra map $\digamma : T(\mathbb{A}^{\mathbb{Q}})\hat\otimes_{\mathbb{Q}}\mathbb{Q}[F] \to \hat{T}(H^{\mathbb{Q}})$ such that $\tilde\theta := \digamma \circ \theta$ is a symplectic expansion of π.*

Proof. We consider the special expansion θ of (π, A) that appears in the proof of Lemma 7.3 starting from a special expansion θ_0 of the free group D. We shall follow the notations of this proof, but we will not specify the algebra map $q : \widehat{T}(\mathbb{D}^{\mathbb{Q}}) \to \widehat{T}(\mathbb{A}^{\mathbb{Q}})$ when using it. Set $a_i := [\alpha_i] \in H^{\mathbb{Q}}$ and $b_i := [\beta_i] \in H^{\mathbb{Q}}$ for $i \in \{1, \ldots, g\}$.

Let $\digamma : T(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F] \to \widehat{T}(H^{\mathbb{Q}})$ be the $\mathbb{Q}$-algebra homomorphism defined by

$$\digamma(a_i) := \Big(\frac{-\mathrm{ad}_{b_i}}{\exp(-\mathrm{ad}_{b_i}) - \mathrm{id}}\Big)(a_i), \quad \digamma(x_i) := \exp(b_i) \tag{10.6}$$

for all $i \in \{1, \ldots, g\}$. Since $\digamma$ preserves the degree-filtrations, it extends continuously to a complete $\mathbb{Q}$-algebra homomorphism $\digamma : T(\mathbb{A}^{\mathbb{Q}})\hat\otimes_{\mathbb{Q}}\mathbb{Q}[F] \to \widehat{T}(H^{\mathbb{Q}})$. We claim that, for an appropriate choice of θ_0, the map $\tilde{\theta} := \digamma \circ \theta$ is a symplectic expansion of π:

(i) We have

$$\begin{aligned} \tilde{\theta}(\alpha_i) &\overset{(7.8)}{=} \digamma(\exp(u_i)\exp(a_i)\exp(-u_i)\otimes 1) \\ &= \digamma(\exp\big(\exp(\mathrm{ad}_{u_i})(a_i)\big)\otimes 1) \\ &= \exp\big(\exp(\mathrm{ad}_{\digamma(u_i)})(\digamma(a_i))\big)\otimes 1; \end{aligned}$$

since u_i is primitive and since $\digamma$ preserves the primitive parts, the element $\tilde{\theta}(\alpha_i)$ of $\widehat{T}(H^{\mathbb{Q}})$ is group-like; besides, the above formula shows that $\log\tilde{\theta}(\alpha_i)$ starts like $\digamma(a_i)$ with a_i in degree 1.

(ii) We have

$$\begin{aligned} \tilde{\theta}(\beta_i) &\overset{(7.9)}{=} \digamma\big(\exp(u_i)\exp(-({}^{x_i}u_i'))\otimes x_i\big) \\ &= \exp(\digamma(u_i))\exp(b_i)\exp(-\digamma(u_i')); \end{aligned}$$

by the same argument as in (i), the tensors $\digamma(u_i)$ and $\digamma(u_i')$ are primitive, so that the element $\tilde{\theta}(\beta_i)$ is group-like; besides, according to (7.4), one can choose the special expansion θ_0 so that the degree-one part of u_i is

$$\frac{1}{2}a_i + \frac{1}{2}\sum_{j>i}(-a_j' + a_j)$$

and is equal to the degree-one part of u_i'; therefore, the above formula shows that $\log\tilde{\theta}(\beta_i)$ starts with b_i in degree 1.

(iii) It follows from (i) and (ii) that $\tilde{\theta}$ is an expansion of π.

(iv) It remains to verify the symplectic condition (10.5):

$$\begin{aligned} \tilde{\theta}(\zeta) &\overset{(7.3)}{=} \digamma\Big(\sum_{i=1}^{g}\big(a_i - (a_i)^{x_i}\big)\Big) \\ &= \sum_{i=1}^{g}\big(\digamma(a_i) - \exp(-b_i)\digamma(a_i)\exp(b_i)\big) \\ &= \sum_{i=1}^{g}\big(\mathrm{id} - \exp(-\mathrm{ad}_{b_i})\big)(\digamma(a_i)) \;=\; -\sum_{i=1}^{g}[a_i, b_i]. \end{aligned}$$

We now prove the injectivity of $\digamma$. Let $P : \widehat{T}(H^{\mathbb{Q}}) \to \widehat{T}(H^{\mathbb{Q}})$ be the endomorphism of complete $\mathbb{Q}$-algebras defined by

$$P(a_i) = \Big(\frac{\exp(-\mathrm{ad}_{b_i}) - \mathrm{id}}{-\mathrm{ad}_{b_i}}\Big)(a_i), \qquad P(b_i) = b_i$$

for all $i \in \{1, \dots, g\}$. Since P induces the identity at the graded level, it is an isomorphism. Thus, the injectivity of $\digamma$ is equivalent to the injectivity of the map $\digamma' := P \circ \digamma$, which is given by $\digamma'(a_i) = a_i$ and $\digamma'(x_i) = \exp(b_i)$.

Let $I = I_F$ denote the augmentation ideal of $\mathbb{Q}[F]$. Consider the filtration $(V_n)_{n\geq 0}$ on $T(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$ induced by the degree-filtration on $T(\mathbb{A}^{\mathbb{Q}})$ and the I-adic filtration on $\mathbb{Q}[F]$:

$$V_n = \sum_{i+j=n} T^{\geq i}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} I^j, \; n \geq 0.$$

Let $T(\mathbb{A}^{\mathbb{Q}})\hat{\hat{\otimes}}_{\mathbb{Q}}\mathbb{Q}[F]$ denote the completion of $T(\mathbb{A}^{\mathbb{Q}})\otimes_{\mathbb{Q}}\mathbb{Q}[F]$ with respect to V. The degree-filtration of $T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]$ is contained in V, i.e. we have

$$T^{\geq n}(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F] \subset V_n,\ n \geq 0.$$

Therefore, the identity induces a $\mathbb{Q}$-linear map $\rho : T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F] \to T(\mathbb{A}^{\mathbb{Q}})\hat{\hat{\otimes}}_{\mathbb{Q}}\mathbb{Q}[F]$. Let $\Upsilon : \widehat{T}(H^{\mathbb{Q}}) \to T(\mathbb{A}^{\mathbb{Q}})\hat{\hat{\otimes}}_{\mathbb{Q}}\mathbb{Q}[F]$ be the unique homomorphism of filtered algebras such that $\Upsilon(a_i) = a_i$ and $\Upsilon(b_i) = \log(x_i) = \sum_{k\geq 1}(-1)^{k+1}(x_i-1)^k/k$. Clearly, we have $\Upsilon \circ F' = \rho$. So, it is enough to prove the injectivity of ρ.

Let $w \in T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]$ with $\rho(w) = 0$. We write w as a (possibly infinite) sum $w = \sum_{m\geq 0} w_m$ with $w_m \in T^m(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$. Fix an integer $k \geq 0$. By assumption on w, we have $\sum_{m=0}^k w_m \in V_{k+1}$. For every $n \geq 0$, the space V_n can also be written as the direct sum

$$V_n = \Big(T^{>n}(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]\Big) \oplus \Big(\bigoplus_{i+j=n} T^i(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} I^j\Big).$$

Hence, for every $m \in \{0,\dots,k\}$, we obtain that w_m belongs to the subspace $T^m(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} I^{k+1-m}$ of $T^m(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \mathbb{Q}[F]$. Now, fixing $m \geq 0$, we get that

$$w_m \in \bigcap_{k>m} \Big(T^m(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} I^{k+1-m}\Big) = T^m(\mathbb{A}^{\mathbb{Q}}) \otimes_{\mathbb{Q}} \bigcap_{k>m} I^{k+1-m} = \{0\}$$

and we conclude that $w = 0$. □

To prove (10.4), we shall also need the diagrammatic description of the conjugation action of the automorphism group on the Lie algebra of special derivations. Recall from §2.2 that $\mathrm{IAut}\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ is the automorphism group of complete Hopf algebra inducing the identity on the associated graded. Recall also that $\mathrm{Der}_+\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ is the Lie algebra of derivations mapping any $x \in F$ to $\widehat{\mathrm{Lie}}(\mathbb{A}^{\mathbb{Q}})\,x$ and mapping $\mathbb{A}^{\mathbb{Q}}$ to $\widehat{\mathrm{Lie}}_{\geq 2}(\mathbb{A}^{\mathbb{Q}})$. Let also $\mathrm{IAut}^{\zeta}(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F])$ be the subgroup of automorphisms fixing $[\zeta] \in \mathbb{A}$ and, similarly, let $\mathrm{Der}_+^{\zeta}(T\big(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ be the Lie subalgebra vanishing on $[\zeta] \in \mathbb{A}$. We can sum up Lemma 2.2, isomorphism (3.5), Proposition 8.2, Proposition 8.4 and isomorphism (9.4) as follows:

$$\begin{tikzcd}
\mathrm{IAut}^{\zeta}\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big) \arrow[r, "\log", "\simeq"'] & \mathrm{Der}_+^{\zeta}\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big) \arrow[r, "\mathrm{res}", "\simeq"'] & \widehat{\mathrm{Der}}_+^{\zeta}(\mathsf{A}_{\bullet}^{\mathbb{Q}}) \arrow[dl, "\mathrm{res}"', "\simeq"] \arrow[d, "\mathrm{res}", "\simeq"'] \\
\widehat{\mathcal{D}} \arrow[r, "\simeq", "\eta"'] & \widehat{D}_+^0 \otimes \mathbb{Q} & \widehat{D}_+^1 \otimes \mathbb{Q}
\end{tikzcd} \tag{10.7}$$

Besides, by transforming beads and leaves in the obvious way, $\mathrm{IAut}\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ acts on the degree-completion of the quotient space $\mathcal{D}'/\mathcal{E} \simeq \mathcal{D}$ introduced in Lemma 9.9. So we get a canonical action of $\mathrm{IAut}\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ on $\widehat{\mathcal{D}}$.

Lemma 10.7. *The canonical action of* $\mathrm{IAut}^{\zeta}\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ *on* $\widehat{\mathcal{D}}$ *corresponds to the conjugation action of* $\mathrm{IAut}^{\zeta}\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ *on* $\mathrm{Der}_+^{\zeta}(T\big(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ *through the isomorphism* $\widehat{\mathcal{D}} \simeq \mathrm{Der}_+^{\zeta}(T\big(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ *described by* (10.7).

Proof. The (left) conjugation action of the automorphism group of the algebra $T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]$ on the Lie algebra of its derivations restricts to an action of the subgroup $\mathrm{IAut}^{\zeta}\big(T(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$ on the Lie subalgebra $\mathrm{Der}_+^{\zeta}(T\big(\mathbb{A}^{\mathbb{Q}})\hat{\otimes}_{\mathbb{Q}}\mathbb{Q}[F]\big)$. Indeed, let $\psi \in \mathrm{IAut}^\zeta\big(T(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$ and let $d \in \mathrm{Der}^\zeta_+(T\big(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$. Setting $\delta := \log(\psi)$, we have $\psi d \psi^{-1} = \exp(\mathrm{ad}_\delta)(d)$. Since δ belongs to $\mathrm{Der}^\zeta_+(T\big(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$, so does $\mathrm{ad}^n_\delta(d)$ for any $n \geq 0$. Therefore, $\psi d \psi^{-1}$ belongs to $\mathrm{Der}^\zeta_+(T\big(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$.

Let $t, \tau \in \widehat{\mathcal{D}}$ correspond to $d, \delta \in \mathrm{Der}^\zeta_+(T\big(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$, respectively, in (10.7). Let $t' := \psi \cdot t$ be the result of the action of ψ on t, and let $d' \in \mathrm{Der}^\zeta_+(T\big(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$ correspond to $t' \in \widehat{\mathcal{D}}$ in (10.7). We claim that

$$t' = \exp(\mathrm{ad}_\tau)(t), \tag{10.8}$$

which implies that $d' = \exp(\mathrm{ad}_\delta)(d) = \psi d \psi^{-1}$ and proves the lemma. By multilinearity and the bead-out relation, we can assume that t consists of a single tree without bead. Then, assume that t has r leaves and number them in an arbitrary way: let $\ell_1, \dots, \ell_r \in \mathbb{A}^\mathbb{Q}$ be the colors of these leaves. Given $\ell'_1, \dots, \ell'_r \in \widehat{\mathrm{Lie}}(\mathbb{A}^\mathbb{Q})$, let $t(\ell'_1, \dots, \ell'_r) \in \widehat{\mathcal{D}}$ denote the series of trees obtained from t by changing each color ℓ_i to ℓ'_i and expanding the leaf (see Lemma 9.9). Then, the claim (10.8) can be reformulated as

$$t\big(\exp(\delta)(\ell_1), \dots, \exp(\delta)(\ell_r)\big) = \exp(\mathrm{ad}_\tau)(t),$$

or, more explicitly, as

$$\sum_{k_1,\dots,k_r \geq 0} \frac{1}{k_1! \cdots k_r!} t\big(\delta^{k_1}(\ell_1), \dots, \delta^{k_r}(\ell_r)\big) = \sum_{n \geq 0} \frac{1}{n!} [\underbrace{\tau, [\tau, \dots [\tau}_{n \text{ times}}, t] \dots]]. \tag{10.9}$$

Next, we observe the following fact by comparing the formulas (9.5) and (9.6). Let E' be a tree with leaves colored by $\widehat{\mathrm{Lie}}(\mathbb{A}^\mathbb{Q})$ and without bead, and let $E \in \widehat{\mathcal{D}}$ be obtained by simultaneous expansions of E' at all leaves. Then $[\tau, E] \in \widehat{\mathcal{D}}$ is the sum of all ways of choosing a leaf of E', applying δ to the color of that leaf, and then expanding at all leaves. It follows from the previous observation that

$$[\underbrace{\tau, [\tau, \dots [\tau}_{n \text{ times}}, t] \dots]] = \sum_{k_1,\dots,k_r \geq 0} \binom{n}{k_1, \dots, k_r} t\big(\delta^{k_1}(\ell_1), \dots, \delta^{k_r}(\ell_r)\big)$$

and (10.9) immediately follows. □

We can now prove formula (10.4).

Proof of Theorem 10.5. Let θ_1 and θ_2 be two special expansions of the free pair (π, A). Then, there is a (unique) automorphism ψ of the complete Hopf algebra $T(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]$ inducing the identity at the graded level and such that $\psi \circ \theta_1 = \theta_2$. On the one hand, using the actions of $\mathrm{IAut}^\zeta\big(T(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$ that are discussed in Lemma 10.7, we have

$$\begin{aligned} \eta\Big(\frac{1}{2}\log\theta_2(u) — \log\theta_2(u)\Big) &= \eta\Big(\frac{1}{2}\psi\big(\log\theta_1(u)\big) — \psi\big(\log\theta_1(u)\big)\Big) \\ &= \psi \circ \eta\Big(\frac{1}{2}\log\theta_1(u) — \log\theta_1(u)\Big) \circ \psi^{-1}, \end{aligned}$$

where the values of η are viewed as elements of $\widehat{D}^0_+ \simeq \mathrm{Der}^\zeta_+(T\big(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$. On the other hand, the definition of the representation $\varrho^{\theta_i} : \mathcal{T} \to \mathrm{Der}^\zeta_+(T\big(\mathbb{A}^\mathbb{Q})\hat{\otimes}_\mathbb{Q}\mathbb{Q}[F]\big)$ implies that

$$\varrho^{\theta_2}(T_{\partial U}) = \psi \circ \varrho^{\theta_1}(T_{\partial U}) \circ \psi^{-1}.$$

Therefore, (10.4) holds for θ_1 if and only if it does for θ_2.

Thus, we can restrict ourselves to a special expansion θ of (π, A) as in Lemma 10.6. Let $\tilde\theta = \digamma\theta$ be the corresponding symplectic expansion of π. By its definition, and when viewed as a 1-cocycle, $\varrho^\theta(T_{\partial U})$ maps $x_i \in F$ $(1 \le i \le g)$ to

$$U_i := \log\Big(\theta\,\widehat{\mathbb{Q}[T_{\partial U}]}\,\theta^{-1}\Big)(x_i)\; x_i^{-1} \in \widehat{\mathrm{Lie}}(\mathbb{A}^{\mathbb{Q}}) \subset T(\mathbb{A}^{\mathbb{Q}})\hat\otimes\mathbb{Q}[F],$$

where $\widehat{\mathbb{Q}[T_{\partial U}]} : \widehat{\mathbb{Q}[\mathsf{A}_*]} \to \widehat{\mathbb{Q}[\mathsf{A}_*]}$ is induced by $T_{\partial U} \in \mathrm{Aut}(\pi, \mathsf{A})$ on the $J_*^{\mathbb{Q}}(\mathsf{A}_*)$-completion of $\mathbb{Q}[\pi]$, and $\theta : \widehat{\mathbb{Q}[\mathsf{A}_*]} \to \hat U(\overline{\mathsf{A}}_*^{\mathbb{Q}}) = T(\mathbb{A}^{\mathbb{Q}})\hat\otimes_{\mathbb{Q}}\mathbb{Q}[F]$ is the continuous extension of θ. We deduce from the definition (10.6) of $\digamma$ that

$$\digamma(U_i) = \log\Big(\tilde\theta\,\widehat{\mathbb{Q}[T_{\partial U}]}\,\tilde\theta^{-1}\Big)(\exp(b_i))\;\exp(-b_i), \tag{10.10}$$

where $\widehat{\mathbb{Q}[T_{\partial U}]} : \widehat{\mathbb{Q}[\pi]} \to \widehat{\mathbb{Q}[\pi]}$ is induced by $T_{\partial U} \in \mathrm{Aut}(\pi)$ on the I-adic completion of $\mathbb{Q}[\pi]$, and $\tilde\theta : \widehat{\mathbb{Q}[\pi]} \to \hat T(H^{\mathbb{Q}})$ is the continuous extension of $\tilde\theta$.

Next, the map $D := \log\big(\tilde\theta\,\widehat{\mathbb{Q}[T_{\partial U}]}\,\tilde\theta^{-1}\big)$, which appears in (10.10), is a derivation of $\hat T(H^{\mathbb{Q}})$, and it can be computed as follows. Indeed, Kawazumi & Kuno gave in [KK14] a closed formula for the logarithm $\log(\widehat{\mathbb{Q}[T_\gamma]})$ of any Dehn twist T_γ, as a derivation of the complete $\mathbb{Q}$-algebra $\widehat{\mathbb{Q}[\pi]}$. Their formula can be stated diagrammatically using any symplectic expansion of π, such as $\tilde\theta$. Let $\tilde\eta : \mathcal{D}(H^{\mathbb{Q}}) \to \mathrm{Der}_+^\omega\big(\mathrm{Lie}(H^{\mathbb{Q}})\big)$ denote the isomorphism (1.8) between the space of trees on $H^{\mathbb{Q}}$ (modulo AS and IHX) and the Lie algebra of symplectic derivations. Then, the Kawazumi–Kuno formula writes

$$\log\big(\tilde\theta\,\widehat{\mathbb{Q}[T_\gamma]}\,\tilde\theta^{-1}\big)\big|_{\widehat{\mathrm{Lie}}(H^{\mathbb{Q}})} = \tilde\eta\Big(\frac{1}{2}\log\tilde\theta(\gamma)\!-\!\!-\!\log\tilde\theta(\gamma)\Big),$$

see [KMT21, §4] for details. Thus, specializing to the meridian $\gamma := \partial U$, we obtain

$$D\big|_{\widehat{\mathrm{Lie}}(H^{\mathbb{Q}})} = \tilde\eta\Big(\frac{1}{2}\digamma(\log\theta(\gamma))\!-\!\!-\!\digamma(\log\theta(\gamma))\Big). \tag{10.11}$$

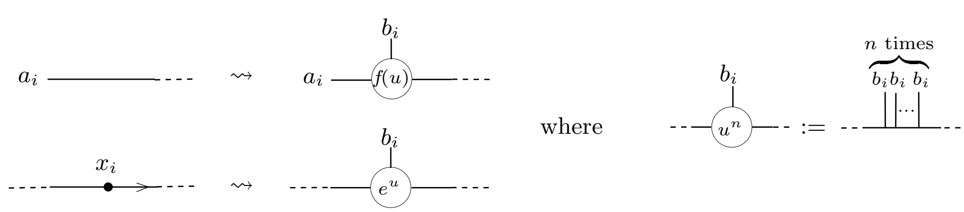
By the usual formula expressing the value of a derivation D on a formal power series (see e.g. [Reu93, Theorem 3.22]), we get

$$\digamma(U_i) \overset{(10.10)}{=} D(\exp(b_i))\,\exp(-b_i) = \big(f^{-1}(\mathrm{ad}_{b_i})\big)\big(D(b_i)\big), \tag{10.12}$$

where

$$f(u) := \frac{u}{\exp(u)-1} \in \mathbb{Q}[[u]].$$

The series of trees $\frac12\digamma(\log\theta(\gamma))\!-\!\!-\!\digamma(\log\theta(\gamma))$ (with leaves colored by $H^{\mathbb{Q}}$) is obtained from the series of trees $S := \frac12\log\theta(\gamma)\!-\!\!-\!\log\theta(\gamma)$ (with leaves colored by $\mathbb{A}^{\mathbb{Q}}$ and beads colored by F) by applying the following operations to all leaves and beads, respectively:



(Here, thanks to the bead-out relation, we assume that all the leaves of S are colored by the $\mathbb{Q}[F]$-basis $(a_1, \dots, a_g)$ of $\mathbb{A}^{\mathbb{Q}}$.) Thus, we can compute $D(b_i)$ from (10.11) and we get the sum

$$\sum_{\ell} \big(f(\mathrm{ad}_{b_i})\big)\big(\digamma(\mathrm{word}(\ell))\big)$$

over all the leaves ℓ of S that are colored by a_i. Therefore, applying (10.12), we obtain that

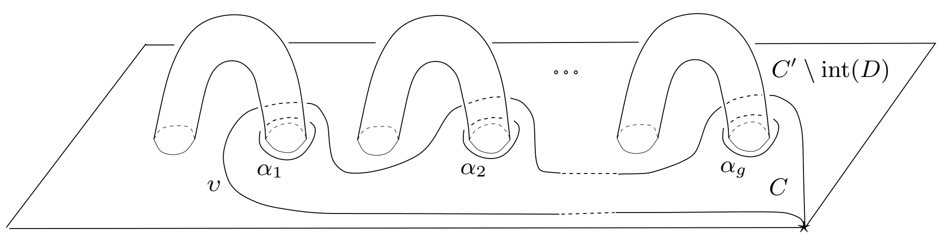
$$\digamma(U_i) = \digamma\Big(\sum_{\ell} \mathrm{word}(\ell)\Big) = -\digamma\big(\eta(S)(x_i)\big).$$

Since $\digamma$ is injective, we conclude that $\varrho^{\theta}(T_{\partial U})(x_i) = U_i = -\eta(S)(x_i)$. Therefore, the 1-cocycles underlying the special derivations $\varrho^{\theta}(T_{\partial U})$ and $-\eta(S)$ are equal. $\square$

Remark 10.8. The presence of a minus sign in (10.4) in contrast with the absence of sign in (10.11) is explained as follows. The identification (8.1) between $\mathbb{A}^{\mathbb{Q}}$ and the dual of the augmentation ideal of $\mathbb{Q}[F]$ (which is involved in the definition of η) is given by $a \mapsto \langle -, a\rangle$ using the homotopy intersection form (A.12) of the handlebody. On the contrary, the identification of $H^{\mathbb{Q}} = H_1(\Sigma;\mathbb{Q})$ with its dual (which is involved in the definition of $\tilde{\eta}$) is given by $h \mapsto \omega(h,-) = -\omega(-,h)$ using the homology intersection form ω of the surface.

10.3. **Example: the pure braid group.** We consider here Oda's embeddings [Oda92] of the g-strand pure braid group PB_g into the mapping class group $\mathcal{M} = \mathcal{M}(\Sigma, \partial\Sigma)$ and, to fit our purposes, we assume here that the image of the embedding is contained in the twist group $\mathcal{T} = \mathcal{T}(V)$. Embeddings of the (framed) pure braid groups into the twist groups, in the context of Johnson filtrations, were also considered in [HV20].

To be more specific, we decompose ∂H as $C \cup_\partial C'$, where C, C' are surfaces of genus 0 such that the disk $D = \partial H \setminus \mathrm{int}(\Sigma)$ is contained in C' and, for a system of curves (α, β) such as (5.4), ∂C consists of the curves $\alpha_1, \dots, \alpha_g$ and an "outer" boundary curve υ:



The inclusion of C into Σ induces a homomorphism $\mathcal{M}(C, \partial C) \to \mathcal{M}$, which is injective. Furthermore, $\mathcal{M}(C, \partial C)$ can be identified with the g-strand framed pure braid group, so that PB_g embeds canonically in $\mathcal{M}(C, \partial C)$ as the group of 0-framed pure braids. Hence, we can view PB_g as a subgroup of $\mathcal{M}$, and it is easily seen that PB_g is actually contained in the twist group $\mathcal{T} = \mathcal{T}(V)$.

The next result relates the lower central series of the pure braid group to the lower central series of the twist group, and to the Johnson filtration of the handlebody group. This is an analogue of [GH02, Theorem 1.1], which deals with the Torelli group and the usual Johnson filtration of the mapping class group.

Theorem 10.9. *For all $k \geq 1$, we have $\Gamma_k PB_g = PB_g \cap \Gamma_k \mathcal{T} = PB_g \cap \mathcal{H}_k$ and the following diagram is commutative:*

$$\begin{tikzcd} \Gamma_k PB_g \arrow[r, hook] \arrow[d, "-\mu_k"'] & \mathcal{H}_k \arrow[d, "\tau_k"] \\ \mathcal{D}_k(A^{\mathbb{Q}}) \arrow[r, tail] & \mathcal{D}_k(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F]). \end{tikzcd} \tag{10.13}$$

In the above diagram, μ_k is the *k-th Milnor homomorphism* which encompasses all Milnor invariants of length $k+1$. Denoting by $A^{\mathbb{Q}}$ the $\mathbb{Q}$-vector space with basis $\{a_1, \dots, a_g\}$, the invariant μ_k takes values in the space

$$\mathcal{D}_k(A^{\mathbb{Q}}) = \frac{\mathbb{Q} \cdot \{\text{node-oriented trees on } A^{\mathbb{Q}}\}}{\text{AS, IHX, multilinearity}}.$$

We now review the definition of this homomorphism. It involves the canonical action of PB_g on the fundamental group $A := \pi_1(C, \star)$, which is the free group generated by $\alpha_1, \dots, \alpha_g$.

Let $t \in PB_g$. Let $\ell_1(t), \dots, \ell_g(t) \in A$ denote the *longitudes* of t, which are uniquely defined by the conditions that $t(\alpha_i) = \ell_i(t) \cdot \alpha_i \cdot \ell_i(t)^{-1} \in A$, and $[\ell_i(t)] \in H_1(A; \mathbb{Z})$ is a $\mathbb{Z}$-linear combination of the $a_j = [\alpha_j]$ for $j \neq i$. Then, for any $k \geq 2$, the following statements are well-known to be equivalent to each other (see e.g. [HM00, Proof of Lemma 16.4]):

(i) t belongs to $\Gamma_k PB_g$,
(ii) for all $x \in A$, $t(x)x^{-1}$ belongs to $\Gamma_{k+1} A$,
(iii) for all $i \in \{1, \dots, g\}$, $\ell_i(t)$ belongs to $\Gamma_k A$.

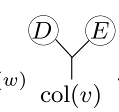
In the sequel, we identify the associated graded of the lower central series of A (with rational coefficients) with the Lie $\mathbb{Q}$-algebra generated by $A^{\mathbb{Q}}$. Assume now that $t \in \Gamma_k PB_g$ and define

$$\mu_k(t) = \sum_{i=1}^{g} a_i \otimes [\ell_i(t)]_k \in A^{\mathbb{Q}} \otimes_{\mathbb{Q}} \mathrm{Lie}_k(A^{\mathbb{Q}}).$$

Since t preserves the boundary component v of C, it follows that $\mu_k(t)$ belongs to the kernel of the Lie bracket of $\mathrm{Lie}(A^{\mathbb{Q}})$. Hence, using the isomorphism (9.2), we can view $\mu_k(t)$ as an element of $\mathcal{D}_k(A^{\mathbb{Q}})$. The resulting map $\mu_k : \Gamma_k PB_g \to \mathcal{D}_k(A^{\mathbb{Q}})$ is a homomorphism and, by the above equivalence "(i)⇔(iii)", we have $\ker \mu_k = \Gamma_{k+1} PB_g$. It is also known (see e.g. [HP03, Prop. 3]) that the map

$$(-\mu_k)_{k\geq 1} : \bigoplus_{k \geq 1} \frac{\Gamma_k PB_g}{\Gamma_{k+1} PB_g} \otimes \mathbb{Q} \longrightarrow \mathcal{D}(A^{\mathbb{Q}})$$

is a homomorphism of graded Lie $\mathbb{Q}$-algebras, if $\mathcal{D}(A^{\mathbb{Q}})$ is endowed with the Lie bracket defined, for any trees D and E, by the formula

(10.14) $$[D, E] = \sum_{v,w} \delta_{\mathrm{col}(v), \mathrm{col}(w)}$$ 

.

Here the sum is over all leaves v and w of D and E, respectively, and the corresponding "branched" tree is obtained by gluing D and E along the half-edges incident to v and w whenever $\mathrm{col}(v) = \mathrm{col}(w)$, the new leaf being then colored by $\mathrm{col}(v)$.

Proof of Theorem 10.9. Let us first prove the injectivity of $\mathcal{D}(A^{\mathbb{Q}}) \to \mathcal{D}(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$. For this, we identify $\mathcal{D}(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$ with the space $\mathcal{D}(\mathbb{A}^{\mathbb{Q}})_{\mathbb{Q}[F]}$ defined at (9.3). Set $S := \{a_1, \dots, a_g\}$. Consider the cartesian product $F \times S$, which, to suggest the canonical left action of F on $F \times S$, we prefer to refer to as

$$F \cdot S := \big\{ f \cdot a_1, \dots, f \cdot a_g \,\big|\, f \in F \big\}.$$

Then, getting rid of the "multilinearity" relations, we can identify $\mathcal{D}(A^{\mathbb{Q}})$ with

$$\mathcal{D}(S) := \frac{\mathbb{Q} \cdot \{\text{node-oriented trees on } S\}}{\text{AS, IHX}},$$

and identify $\mathcal{D}(\mathbb{A}^{\mathbb{Q}})_{\mathbb{Q}[F]}$ with

$$\mathcal{D}(F \cdot S)_F := \frac{\mathbb{Q} \cdot \{\text{node-oriented trees on } F \cdot S\}}{\text{AS, IHX, translation}},$$

where, for any $f \in F$, the "translation" relation identifies any tree on $F \cdot S$ with the same tree where f as acted on each leaf. (This last identification is allowed since $\mathbb{A}^{\mathbb{Q}}$ is free on $a_1, \dots, a_g$ as a $\mathbb{Q}[F]$-module.) We now fix a degree $k \geq 1$. The diagonal action of F on $(F \cdot S)^{k+1}$ commutes with the canonical action of the symmetric group $\mathfrak{S}_{k+1}$. Let Q be the corresponding double quotient set. An element of Q can be assigned to any tree of degree k on $F \cdot S$. Thus, $\mathcal{D}(F \cdot S)_F$ splits as a direct sum over Q and, clearly, $\mathcal{D}(S)$ is there the sum of the direct summands corresponding to the double cosets that have a (unique) representative in S^{k+1}. This proves the injectivity of the map $\mathcal{D}_k(A^{\mathbb{Q}}) \to \mathcal{D}_k(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$ for every $k \geq 1$.

Since $PB_g \subset \mathcal{T}$, we have $\Gamma_k PB_g \subset PB_g \cap \Gamma_k \mathcal{T} \subset PB_g \cap \mathcal{H}_k$. Hence, we only have to prove the inclusion $PB_g \cap \mathcal{H}_k \subset \Gamma_k PB_g$. But, since we have $\Gamma_{k+1} PB_g = \ker \mu_k$ and $\mathcal{H}_{k+1} = \ker \tau_k$, the inclusion $PB_g \cap \mathcal{H}_{k+1} \subset \Gamma_{k+1} PB_g$ follows from (10.13) by induction on k.

Therefore, it only remains to prove the commutativity of (10.13). Recall that PB_g is generated by the "elementary" pure braids t_{ij} (for $i \neq j$) that "clasp" the i-th and the j-th strands in front of the other strands. Specifically, we have

$$t_{ij} = T_{\gamma_{ij}} T_{\alpha_i}^{-1} T_{\alpha_j}^{-1},$$

where γ_{ij} is a simple closed curve "encircling" α_i and α_j. We have $\mu_1(t_{ij}) = a_i$—a_j and, according to Proposition 10.1, we have

$$\tau_1(t_{ij}) = -\frac{1}{2}(a_i + a_j)\text{—}(a_i + a_j) + \frac{1}{2} a_i\text{—}a_i + \frac{1}{2} a_j\text{—}a_j = -a_i\text{—}a_j.$$

Therefore, the diagram (10.13) is commutative for $k = 1$. Besides, by comparing formulas (10.14) and (9.6), we observe that the map $\mathcal{D}_k(A^{\mathbb{Q}}) \to \mathcal{D}_k(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$ preserves the Lie brackets. The conclusion follows since, for arbitrary $k \geq 1$, the abelian group $\Gamma_k PB_g / \Gamma_{k+1} PB_g$ is generated by iterated commutators of length k in the t_{ij}'s. □

11. Connections and prospects

In this concluding section, we mention some relations between our approach and some other approaches to the handlebody group, and also briefly describe some new perspectives that the present paper opens up.

11.1. **Restriction of the usual Johnson filtration to the handlebody group.** Another natural filtration of the handlebody group $\mathcal{H}$ is the restriction $(\mathcal{M}_k \cap \mathcal{H})_{k\geq 0}$ of the usual Johnson filtration $(\mathcal{M}_k)_{k\geq 1}$ of the mapping class group $\mathcal{M}$, which was reviewed in §1.1. For instance, the first term $\mathcal{H} \cap \mathcal{M}_1$ is the intersection of the handlebody group with the Torelli group, see [Pi09, Om19] for a generating system.

This approach, which is evoked in [Hen18, §7] and considered e.g. in [Fa23], is quite different from ours. Nevertheless, our Johnson filtration of $\mathcal{H}$ is contained in $(\mathcal{T} \cap \mathcal{M}_k)_{k\geq 1}$, and our Johnson homomorphisms determine the usual ones. Specifically, we have

$$\mathcal{H}_k \ \subset\ \mathcal{M}_{k-1} \cap \mathcal{H}, \quad \text{for all } k \geq 1$$

and, for $f \in \mathcal{H}_k$ with $k \geq 2$, the usual Johnson homomorphism $\tau^{\mathrm{usual}}_{k-1}(f) \in \mathcal{D}_{k-1}(H^{\mathbb{Q}})$ is obtained from $\tau_k(f) \in \mathcal{D}_k(\mathbb{A}^{\mathbb{Q}}, \mathbb{Q}[F])$ by ignoring beads and transforming the colors of leaves through the homomorphism $\mathbb{A} \to H$ (induced by the inclusion of A in π). More generally, it would be interesting to relate our Johnson filtration of the handlebody group to the “double Johnson filtration” that was introduced in [HV20].

11.2. **Relative weight filtration for the handlebody group.** In [Ha08], Hain considers the “relative weight filtration” on (the relative completion of) the mapping class group with respect to a finite set of pairwise-disjoint simple closed curves on the surface. When those curves are given by a pants decomposition of the surface, this filtration depends only on the handlebody underlying the pants decomposition. Furthermore, the 0-th and 1-st terms of this filtration are the corresponding handlebody group and twist group, respectively.

It would be interesting to compare Hain’s relative weight filtration of the handlebody group to our Johnson filtration. Indeed, combining the strictness and exactness of the former with the explicit algebraic descriptions of the latter may be useful in the study of handlebody groups.

11.3. **Abelianization of the twist group.** In contrast with the Torelli group [Jo85], the structure of the abelianization of $\mathcal{T}$ is not well understood. The first step in the understanding of this structure would be to determine the image of the first Johnson homomorphism $\tau_1^0 : \mathcal{T} \to D_1^0$ or, equivalently, the image of the Magnus representation $\mathrm{Mag} : \mathcal{T} \to \mathrm{Mat}(g \times g; \mathbb{Z}[F])$.

The second step would be to decide whether the abelianization of $\mathcal{T}$ is torsion-free. In fact, computing the rational abelianization of $\mathcal{T}$ is already a challenge, and it is necessary for the computation of its Malcev Lie algebra.

11.4. **Images of the Johnson homomorphisms and trace maps.** A more general problem for a further study of the filtration $(\mathcal{H}_k)_{k\geq 1}$ would be to determine the images of the Johnson homomorphisms in any degree $k \geq 1$. In the case of the usual Johnson filtration $(\mathcal{M}_k)_{k\geq 1}$, reviewed in §1.1, this problem has not been solved yet, but there exist “divergence” 1-cocycles on the Lie algebra $\mathrm{Der}^{\omega}_{+}(\mathrm{Lie}(H))$ which are known to vanish on $\overline{\tau}_+(\overline{\mathcal{M}}_+)$. Such 1-cocycles include the Morita trace [Mo93] and the Enomoto–Satoh trace [ES14]. It is important to construct analogues of those 1-cocycles for the Johnson filtration of the handlebody group.

11.5. **Tree-level of the extended Kontsevich integral.** The handlebody groups are the groups of automorphisms in the category of "bottom tangles in handlebodies" [Ha06]. The Kontsevich integral (originally defined for tangles in balls) was extended in [HM21] to a functor Z from this category to the category of "Jacobi diagrams in handlebodies". Thus, we obtain from Z new diagrammatic representations of the handlebody group $\mathcal{H}$ in any genus $g \geq 1$. These might be useful for the difficult problem of determining the Malcev Lie algebra of $\mathcal{T}$.

In a future work, it will be shown that the tree-level of $Z|_{\mathcal{T}}$ (which consists in ignoring non-acyclic Jacobi diagrams) is equivalent to the "infinitesimal" action ϱ^θ of $\mathcal{T}$ on the free pair (π, A). Here θ is a certain special expansion of (π, A), which is itself defined from the extended Kontsevich integral. It follows that, for every $k \geq 1$, the degree k part of the tree-level of $Z|_{\mathcal{H}_k}$ is equivalent to τ_k.

Appendix A. Intersection operations in a handlebody

In this appendix, we describe several intersection operations in a handlebody.

A.1. **The homotopy intersection form of a surface.** We start by reviewing Turaev's homotopy intersection form of a surface [Tu78]. This form determines the homology intersection forms of Σ with arbitrary twisted coefficients, and it is also implicit in Papakyariakopoulos' work [Pa75].

Let Σ be a compact connected oriented surface with one boundary component. Its fundamental group $\pi = \pi_1(\Sigma, \star)$ is based at a point $\star \in \partial\Sigma$. Let

$$\eta : \mathbb{Z}[\pi] \times \mathbb{Z}[\pi] \longrightarrow \mathbb{Z}[\pi]$$

be the $\mathbb{Z}$-bilinear pairing that maps any pair $(x, y) \in \pi \times \pi$ to

$$\eta(x,y) = \sum_{p \in X \cap Y} \varepsilon_p(X,Y) \ \left[(\overline{\partial\Sigma})_{\star\bullet} X_{\bullet p} Y_{p\star} \right]. \tag{A.1}$$

Here $\bullet$ ($\neq \star$) is a second base-point in $\partial\Sigma$, X is a loop based at $\bullet$ such that $(\overline{\partial\Sigma})_{\star\bullet}\, X\, (\partial\Sigma)_{\bullet\star}$ represents x, Y is a loop based at $\star$ representing y, and X and Y meet transversely in a finite set of double points. The operation η is a *Fox pairing* in the sense that it is a left *Fox derivative* in its first argument:

$$\eta(xx', y) = x\, \eta(x', y) + \eta(x, y)\, \varepsilon(x') \quad (\text{for all } x, x', y' \in \mathbb{Z}[\pi]) \tag{A.2}$$

and right *Fox derivative* in its second argument:

$$\eta(x, yy') = \eta(x, y)\, y' + \varepsilon(y)\, \eta(x, y') \quad (\text{for all } x, y, y' \in \mathbb{Z}[\pi]), \tag{A.3}$$

where $\varepsilon : \mathbb{Z}[\pi] \to \mathbb{Z}$ denotes the augmentation map. (See [MT14, §7] for details.) Observe that η is "almost skew-symmetric":

$$\forall u, v \in \pi, \quad \eta(u,v) = -u\, \overline{\eta(v,u)}\, v - (u-1)(v-1) \tag{A.4}$$

The Fox pairing η is determined by its values on a basis of π. For instance, the matrix of η in a basis (α, β) of type (5.4) is

$$E = \left(\begin{array}{c|c} E_{\alpha\alpha} & E_{\alpha\beta} \\ \hline E_{\beta\alpha} & E_{\beta\beta} \end{array} \right) \in \mathrm{Mat}(2g \times 2g; \mathbb{Z}[\pi]), \tag{A.5}$$

where

$$(E_{\alpha\alpha})_{i,j} = \begin{cases} \alpha_i - 1 & (i=j), \\ P(\alpha_i,\alpha_j) & (i>j), \\ 0 & (i<j), \end{cases} \qquad (E_{\alpha\beta})_{i,j} = \begin{cases} \alpha_i + \beta_i - 1 & (i=j), \\ P(\alpha_i,\beta_j) & (i>j), \\ 0 & (i<j), \end{cases}$$

$$(E_{\beta\alpha})_{i,j} = \begin{cases} -1 & (i=j), \\ P(\beta_i,\alpha_j) & (i>j), \\ 0 & (i<j), \end{cases} \qquad (E_{\beta\beta})_{i,j} = \begin{cases} \beta_i - 1 & (i=j), \\ P(\beta_i,\beta_j) & (i>j), \\ 0 & (i<j), \end{cases}$$

with $P(x,y) = -(x-1)(y-1)$. (See [Mo93, §5] or [Pe06, Lemma 2.4] for a similar computation.)

A.2. **The intersection double bracket of a surface.** We now review a variant of the homotopy intersection form η, which was considered in [MT14]. Define a $\mathbb{Z}$-linear map

$$\{\!\{-,-\}\!\} : \mathbb{Z}[\pi] \otimes \mathbb{Z}[\pi] \longrightarrow \mathbb{Z}[\pi] \otimes \mathbb{Z}[\pi],$$

by

$$\forall a,b \in \mathbb{Z}[\pi], \quad \{\!\{a,b\}\!\} = b' \, \overline{\big(\eta(a'',b'')\big)'} \, a' \otimes \big(\eta(a'',b'')\big)'', \tag{A.6}$$

where we use Sweedler's notation for the coproduct of $\mathbb{Z}[\pi]$. The pairing η can be recovered from $\{\!\{-,-\}\!\}$ by the identity $\eta = (\varepsilon \otimes \mathrm{id}) \circ \{\!\{-,-\}\!\}$. Note that, with the notations of (A.1), we have

$$\forall x,y \in \pi, \quad \{\!\{x,y\}\!\} = \sum_{p \in X \cap Y} \varepsilon_p(X,Y) \ \left[Y_{\star p} X_{p\bullet} (\partial\Sigma)_{\bullet\star}\right] \otimes \left[(\overline{\partial\Sigma})_{\star\bullet} X_{\bullet p} Y_{p\star}\right]. \tag{A.7}$$

Properties (A.2)–(A.3) imply that the operation $\{\!\{-,-\}\!\}$ is a biderivation in the following sense:

$$\forall a,b,c \in \mathbb{Z}[\pi], \quad \{\!\{a,bc\}\!\} = b\,\{\!\{a,c\}\!\}^\ell \otimes \{\!\{a,c\}\!\}^r + \{\!\{a,b\}\!\}^\ell \otimes \{\!\{a,b\}\!\}^r c, \tag{A.8}$$

$$\forall a,b,c \in \mathbb{Z}[\pi], \quad \{\!\{ab,c\}\!\} = \{\!\{b,c\}\!\}^\ell \otimes a\,\{\!\{b,c\}\!\}^r + \{\!\{a,c\}\!\}^\ell\, b \otimes \{\!\{a,c\}\!\}^r. \tag{A.9}$$

Besides, the "skew-symmetry" (A.4) of η implies the following:

$$\forall a,b \in \mathbb{Z}[\pi], \quad \{\!\{a,b\}\!\} = -\{\!\{b,a\}\!\}^r \otimes \{\!\{b,a\}\!\}^\ell - ba \otimes 1 - 1 \otimes ab + b \otimes a + a \otimes b. \tag{A.10}$$

Furthermore, according to [MT14, (7.2.12)], the operation $\{\!\{-,-\}\!\}$ satisfies the following "quasi-Jacobi" identity in $\mathbb{Z}[\pi]^{\otimes 3}$:

$$\begin{aligned} \forall a,b,c \in \mathbb{Z}[\pi], \qquad & \Big\{\!\!\Big\{a, \{\!\{b,c\}\!\}^\ell\Big\}\!\!\Big\} \otimes \{\!\{b,c\}\!\}^r - \{\!\{a,c\}\!\}^l \otimes \{\!\{b, \{\!\{a,c\}\!\}^r\}\!\} \\ & - \Big\{\!\!\Big\{\{\!\{a,b\}\!\}^\ell, c\Big\}\!\!\Big\}^\ell \otimes \{\!\{a,b\}\!\}^r \otimes \Big\{\!\!\Big\{\{\!\{a,b\}\!\}^\ell, c\Big\}\!\!\Big\}^r \\ = \ & \{\!\{a,c\}\!\}^\ell \otimes 1 \otimes b\,\{\!\{a,c\}\!\}^r - \{\!\{a,c\}\!\}^\ell \otimes b \otimes \{\!\{a,c\}\!\}^r. \end{aligned} \tag{A.11}$$

Remark A.1. A slight modification of the operation $\{\!\{-,-\}\!\}$ translates the properties from (A.8) to (A.11) into the axioms of "quasi-Poisson double bracket" in the sense of Van den Bergh [VdB08]. See [MT14].

A.3. **The homotopy intersection form of a handlebody.** We now view Σ as the boundary of a handlebody V, with the interior of disk D removed. Thus we have $\partial V = \Sigma \cup D$.

Let $\varpi : \pi \to F$ be the canonical map onto $F := \pi_1(V,\star)$. Set $\mathsf{A} := \ker \varpi$ and $\mathbb{A} := \mathsf{A}_{\mathrm{ab}}$. Let $\mathbb{A}^r$ denote $\mathbb{A}$ with the right $\mathbb{Z}[F]$-action induced by the right conjugation of π on A. Let I_F denote the augmentation ideal of $\mathbb{Z}[F]$, which we regard as a (left) $\mathbb{Z}[F]$-module.

Proposition A.2. *The homotopy intersection form η of Σ induces a map $\langle -,- \rangle : \mathbb{Z}[F] \times \mathbb{A} \to \mathbb{Z}[F]$, which restricts to a non-singular $\mathbb{Z}[F]$-bilinear map*

$$\langle -,- \rangle : I_F \times \mathbb{A}^r \longrightarrow \mathbb{Z}[F]. \tag{A.12}$$

The latter corresponds (via canonical isomorphisms) to the homology intersection pairing

$$H_1(V,D;\mathbb{Z}[F]) \times H_2(V,\Sigma;\mathbb{Z}[F]) \longrightarrow \mathbb{Z}[F] \tag{A.13}$$

of V with coefficients twisted by the canonical homomorphism $F = \pi_1(V,\star) \to \mathbb{Z}[F]$.

Proof. We denote by the same letter $\varpi : \mathbb{Z}[\pi] \to \mathbb{Z}[F]$ the ring homomorphism induced by $\varpi : \pi \to F$. It follows from (A.3) that the restriction of $\varpi \circ \eta$ to $\mathbb{Z}[\pi] \times \mathsf{A}$ is additive in its second argument, so that it induces a $\mathbb{Z}$-bilinear map $\tilde{\eta} : \mathbb{Z}[\pi] \times \mathbb{A} \to \mathbb{Z}[F]$. Another application of (A.3) shows that

$$\forall x \in \pi,\ \forall a \in \mathsf{A}, \quad \varpi\eta\big(-, x^{-1}ax\big) = \varpi\eta(-,a) \cdot \varpi(x), \tag{A.14}$$

hence $\tilde{\eta} : \mathbb{Z}[\pi] \times \mathbb{A}^r \to \mathbb{Z}[F]$ is $\mathbb{Z}[F]$-linear in its second argument.

Let J be the kernel of $\varpi : \mathbb{Z}[\pi] \to \mathbb{Z}[F]$. To see that $\tilde{\eta}$ factors through a map $\langle -,- \rangle : \mathbb{Z}[F] \times \mathbb{A} \to \mathbb{Z}[F]$, it suffices to show that

$$\tilde{\eta}(J, \mathbb{A}) = 0. \tag{A.15}$$

Moreover, since we have $J = \mathbb{Z}[\pi]\, I_{\mathsf{A}}$ where $I_{\mathsf{A}} = \ker(\epsilon : \mathbb{Z}[\mathsf{A}] \to \mathbb{Z})$, it is enough to prove that $\tilde{\eta}(I_{\mathsf{A}}, \mathbb{A}) = 0$. The group A being normally generated by $\alpha_1, \dots, \alpha_g$ in π, the subset I_{A} is $\mathbb{Z}$-spanned by $x(\alpha_i - 1)x^{-1}$ for all $x \in \pi$ and $i = 1, \dots, g$. But, similarly to (A.14), we have

$$\forall x \in \pi,\ \forall a \in \mathsf{A}, \quad \varpi\eta(xax^{-1}, -) = \varpi(x) \cdot \varpi\eta(a,-). \tag{A.16}$$

Thus, (A.15) follows since $\varpi\eta(\alpha_i, \alpha_j) = 0$ for any $i,j \in \{1, \dots, g\}$.

The restricted map $\langle -,- \rangle : I_F \times \mathbb{A}^r \to \mathbb{Z}[F]$ is also $\mathbb{Z}[F]$-linear in its first argument because of (A.2). To justify its non-singularity, it suffices to compute it in the basis $(x_i - 1)_i$ of I_F and in the basis $([\alpha_j])_j$ of $\mathbb{A}$:

$$\langle x_i - 1, [\alpha_j] \rangle = \varpi\eta(\beta_i, \alpha_j) = -\delta_{ij}. \tag{A.17}$$

Thus the matrix of $\langle -,- \rangle$ in the above bases is $-I_g$, which is invertible.

We prove the second statement, which gives a 3-dimensional interpretation to the pairing $\langle -,- \rangle$. The connecting map in the long exact sequence of the pair (V,D) gives an injection $\partial_* : H_1(V,D;\mathbb{Z}[F]) \to H_0(D;\mathbb{Z}[F]) \simeq \mathbb{Z}[F]$ with image I_F. Hence we get a canonical isomorphism

$$H_1(V,D;\mathbb{Z}[F]) \simeq I_F. \tag{A.18}$$

Besides, the connecting map of the triple $(V, \Sigma, \star)$ gives an injective homomorphism $\partial_* : H_2(V, \Sigma; \mathbb{Z}[F]) \to H_1(\Sigma, \star; \mathbb{Z}[F])$ whose image coincides with

$$\ker\Big(\mathrm{incl}_* : \underbrace{H_1(\Sigma, \star; \mathbb{Z}[F])}_{\simeq I_\pi \otimes_{\mathbb{Z}[\pi]} \mathbb{Z}[F]} \longrightarrow \underbrace{H_1(V, \star; \mathbb{Z}[F])}_{\simeq I_F}\Big).$$

It is easily checked that the map $I_{\mathsf{A}} \to I_\pi \otimes_{\mathbb{Z}[\pi]} \mathbb{Z}[F]$ defined by $x \mapsto x \otimes 1$ induces an isomorphism between $\mathbb{A} \simeq I_{\mathsf{A}}/I_{\mathsf{A}}^2$ and this kernel. Hence we get a canonical isomorphism

$$H_2(V, \Sigma; \mathbb{Z}[F]) \simeq \mathbb{A}^r. \tag{A.19}$$

That the pairings (A.12) and (A.13) correspond to each other through the isomorphisms (A.18) and (A.19) follows immediately from the computation (A.17). $\square$

Since $J = \ker(\varpi : \mathbb{Z}[\pi] \to \mathbb{Z}[F])$ is an ideal, we deduce from (A.6) and (A.15) that the composition $(\varpi \otimes \varpi) \{\!\{-, -\}\!\}$ induces a linear map

$$\Theta : \mathbb{Z}[F] \otimes \mathbb{A} \longrightarrow \mathbb{Z}[F] \otimes \mathbb{Z}[F] \tag{A.20}$$

which is equivalent to the pairing $\langle -, - \rangle : \mathbb{Z}[F] \times \mathbb{A} \to \mathbb{Z}[F]$. Indeed, we have

$$\begin{array}{rrcl} \forall x \in \mathbb{Z}[F], \forall a \in \mathbb{A}, & \Theta(x, a) & = & \overline{\langle x'', a \rangle'}\, x' \otimes \langle x'', a \rangle'' \\ \text{and, conversely,} & \langle x, a \rangle & = & \varepsilon\left(\Theta(x, a)^\ell\right) \otimes \Theta(x, a)^r. \end{array} \tag{A.21}$$

Proposition A.3. *The map Θ has the following properties:*

$$\forall x, y \in \mathbb{Z}[F],\ \forall a \in \mathbb{A},\ \Theta(xy, a) = \Theta(y, a)^\ell \otimes x \Theta(y, a)^r + \Theta(x, a)^\ell y \otimes \Theta(x, a)^r, \tag{A.22}$$

$$\forall f \in F,\ \forall x \in \mathbb{Z}[F],\ \forall a \in \mathbb{A},\quad \Theta\big(x, {}^f a\big) = f \Theta(x, a)^\ell \otimes \Theta(x, a)^r f^{-1}, \tag{A.23}$$

$$\forall x \in \mathbb{Z}[F],\ \forall a \in \mathbb{A},\quad \Theta(\overline{x}, a) = -\overline{\Theta(x, a)^r} \otimes \overline{\Theta(x, a)^\ell}. \tag{A.24}$$

Proof. The identity (A.22) is a direct application of (A.9), while (A.23) follows from (A.21) and the $\mathbb{Z}[F]$-linearity of $\langle -, - \rangle$ in its second argument:

$$\begin{aligned} \Theta\big(x, {}^f a\big) &= \overline{\langle x'', a^{f^{-1}} \rangle'} x' \otimes \langle x'', a^{f^{-1}} \rangle'' \\ &= \overline{\big(\langle x'', a \rangle f^{-1}\big)'} x' \otimes \big(\langle x'', a \rangle f^{-1}\big)'' \;=\; f \Theta(x, a)^\ell \otimes \Theta(x, a)^r f^{-1}. \end{aligned}$$

Property (A.24) follows from the identity $\{\!\{\overline{u}, \overline{v}\}\!\} = \overline{\{\!\{u, v\}\!\}^r} \otimes \overline{\{\!\{u, v\}\!\}^\ell}$ $(u, v \in \mathbb{Z}[\pi])$, which can be checked using (A.7). $\square$

A.4. **The intersection operation Ψ.** We now derive another operation Ψ from the homotopy intersection form $\eta : \mathbb{Z}[\pi] \times \mathbb{Z}[\pi] \to \mathbb{Z}[\pi]$.

Recall that $J = \ker(\varpi : \mathbb{Z}[\pi] \to \mathbb{Z}[F])$. The following lemma refines the isomorphism (2.3) in degree 1 to integral coefficients.

Lemma A.4. *There is an isomorphism of abelian groups*

$$\gamma : \mathbb{Z}[F] \otimes \mathbb{A} \longrightarrow J/J^2$$

defined by $\gamma(\varpi(x) \otimes [a]) = [x\,(a - 1)]$ for any $x \in \mathbb{Z}[\pi]$ and $a \in \mathsf{A}$.

Proof. It is easily verified that the map γ is well-defined. Let B be a subgroup of π that maps isomorphically onto F by ϖ. Then, we can write any $j \in J$ uniquely as a finite sum $j = \sum_{b \in B} b\, a_b(j)$ with $a_b(j) \in I_{\mathsf{A}}$. Thus, we have a homomorphism

$$\rho : J \longrightarrow \mathbb{Z}[F] \otimes (I_{\mathsf{A}}/I_{\mathsf{A}}^2), \ j \longmapsto \sum_{b \in B} \varpi(b) \otimes [a_b(j)]$$

and we easily check that $\rho(J^2)$ is trivial. Clearly, the resulting homomorphism $\rho : J/J^2 \to \mathbb{Z}[F] \otimes (I_{\mathsf{A}}/I_{\mathsf{A}}^2) \simeq \mathbb{Z}[F] \otimes \mathbb{A}$ is the inverse to γ. □

To define our last intersection operation Ψ, recall from (A.15) that $\eta(\mathsf{A}, \mathsf{A}) \subset J$.

Proposition A.5. *There is a unique $\mathbb{Z}$-bilinear map Ψ that fits into the following commutative diagram:*

$$\begin{tikzcd} \mathsf{A} \times \mathsf{A} \arrow[r, "\eta"] \arrow[d, two heads] & J \arrow[r, two heads] & J/J^2 \\ \mathbb{A} \times \mathbb{A} \arrow[rr, "\Psi"] & & \mathbb{Z}[F] \otimes \mathbb{A} \arrow[u, "\gamma"', "\simeq"] \end{tikzcd} \tag{A.25}$$

Furthermore, Ψ has the following properties:

$$\forall a \in \mathbb{A}, \quad \Psi(a, [\zeta]) = 1 \otimes a, \quad \text{where } \zeta \in \mathsf{A} \text{ is the homotopy class of } \partial\Sigma. \tag{A.26}$$

$$\forall x \in F,\ \forall a, b \in \mathbb{A}, \quad \Psi({}^x a, b) = x\Psi(a,b)^\ell \otimes \Psi(a,b)^r - \Theta(x,b)^r \otimes {}^{\Theta(x,b)^\ell} a. \tag{A.27}$$

$$\forall y \in F,\ \forall a, b \in \mathbb{A}, \quad \Psi(a, {}^y b) = \Psi(a,b)^\ell y^{-1} \otimes {}^y(\Psi(a,b)^r) - \overline{\langle y, a \rangle} \otimes {}^y b. \tag{A.28}$$

$$\forall a, b \in \mathbb{A}, \qquad \Psi(b,a) = \overline{\Psi(a,b)^{\ell'}} \otimes {}^{\Psi(a,b)^{\ell''}}\big(\Psi(a,b)^r\big). \tag{A.29}$$

$$\begin{aligned} \forall a, b, c \in \mathbb{A}, \qquad & \Psi(b,a)^\ell \otimes \Psi(\Psi(b,a)^r, c)^\ell \otimes \Psi(\Psi(b,a)^r, c)^r \\ = \quad & \Psi(b, \Psi(a,c)^r)^\ell\, \overline{\Psi(a,c)^{\ell'}} \otimes \Psi(a,c)^{\ell''} \otimes \Psi(b, \Psi(a,c)^r)^r \\ & -\Theta(\Psi(b,c)^\ell, a)^r \otimes \Theta(\Psi(b,c)^\ell, a)^\ell \otimes \Psi(b,c)^r \\ & -\overline{\langle \Psi(a,c)^{\ell'}, b \rangle} \otimes \Psi(a,c)^{\ell''} \otimes \Psi(a,c)^r. \end{aligned} \tag{A.30}$$

$$\begin{aligned} \forall a, b, c \in \mathbb{A}, \qquad & \Psi(a,c)^\ell \otimes \Psi(b, \Psi(a,c)^r)^\ell \otimes \Psi(b, \Psi(a,c)^r)^r \\ = \quad & \Psi(\Psi(b,a)^r, c)^{\ell'} \otimes \Psi(b,a)^\ell\, \Psi(\Psi(b,a)^r, c)^{\ell''} \otimes \Psi(\Psi(b,a)^r, c)^r \\ & +\overline{\langle \Psi(b,c)^{\ell'}, a \rangle}\, \Psi(b,c)^{\ell''} \otimes \Psi(b,c)^{\ell'''} \otimes \Psi(b,c)^r \\ & +\Psi(a,c)^{\ell'} \otimes \overline{\langle \Psi(a,c)^{\ell''}, b \rangle}\, \Psi(a,c)^{\ell'''} \otimes \Psi(a,c)^r. \end{aligned} \tag{A.31}$$

Proof. Let $q : J \to J/J^2$ be the projection. For any $a, b, c \in \mathsf{A}$, we have

$$\eta(ab, c) = \eta(b,c) + (a-1)\eta(b,c) + \eta(a,c) \equiv \eta(b,c) + \eta(a,c) \mod J^2,$$
$$\eta(a, bc) = \eta(a,b) + \eta(a,b)(c-1) + \eta(a,c) \equiv \eta(a,b) + \eta(a,c) \mod J^2,$$

which shows that the map $q\eta : \mathsf{A} \times \mathsf{A} \to J/J^2$ factors through the canonical projection $\mathsf{A} \times \mathsf{A} \to \mathbb{A} \times \mathbb{A}$ to give a $\mathbb{Z}$-bilinear pairing. This shows the existence (and uniqueness) of the pairing Ψ.

We have $\eta(a, \zeta) = a - 1$ for any $a \in \mathsf{A}$, which proves (A.26). Let $x \in \pi$ and $a, b \in \mathsf{A}$; then (A.27) is proved as follows:

$$\eta({}^x a, b) \ = \ \eta(xax^{-1}, b) \ = \ xa\eta(x^{-1}, b) + x\eta(a,b) + \eta(x,b)$$

$$\begin{aligned} &= (1 - xax^{-1})\eta(x,b) + x\eta(a,b) \\ &= -\eta(x,b)'\,\overline{\eta(x,b)''}x(a-1)x^{-1}\eta(x,b)''' + x\eta(a,b). \end{aligned}$$

Let $y \in \pi$ and $a, b \in \mathsf{A}$; then (A.28) is proved as follows:

$$\begin{aligned} \eta(a, {}^y b) \; = \; \eta(a, yby^{-1}) \;\; &= \;\; \eta(a, yb)y^{-1} + \eta(a, y^{-1}) \\ &= \;\; \eta(a,y)(b-1)y^{-1} + \eta(a,b)y^{-1} \\ &\overset{(A.4)}{\equiv} \;\; -\overline{\eta(y,a)}y(b-1)y^{-1} + \eta(a,b)y^{-1} \mod J^2. \end{aligned}$$

Identity (A.29) follows from

$$q\eta(b,a) \overset{(A.4)}{=} -\overline{q\eta(a,b)} \mod J^2 \quad (a,b \in \mathsf{A})$$

and the following observation: through the isomorphism γ, the involution of J/J^2 induced by the antipode of $\mathbb{Z}[\pi]$ corresponds to the involution $(x \otimes a \mapsto -\overline{x'} \otimes {}^{x''}a)$ of $\mathbb{Z}[F] \otimes \mathbb{A}$.

It now remains to prove (A.30) and (A.31). By applying the map $\varepsilon \otimes \mathrm{id}_{\mathbb{Z}[\pi]} \otimes \mathrm{id}_{\mathbb{Z}[\pi]}$ to (A.11), we obtain the following identity in $\mathbb{Z}[\pi]^{\otimes 2}$:

$$\text{(A.32)}\ \forall a,b,c \in \mathbb{Z}[\pi], \qquad \begin{aligned} &\eta\big(a, \{\!\{b,c\}\!\}^{\ell}\big) \otimes \{\!\{b,c\}\!\}^{r} - \{\!\{b, \eta(a,c)\}\!\} \\ &- \{\!\{a,b\}\!\}^{r} \otimes \eta\big(\{\!\{a,b\}\!\}^{\ell}, c\big) \; = \; 1 \otimes b\,\eta(a,c) - b \otimes \eta(a,c). \end{aligned}$$

Since we have $J = \mathbb{Z}[\pi]\, I_{\mathsf{A}}$ and $\eta(\mathsf{A},\mathsf{A}) \subset J$, we have $\eta(J,J) \subset J$. Thus $q\eta$ induces a $\mathbb{Z}$-bilinear map $\eta_J : (J/J^2) \times (J/J^2) \to J/J^2$. It also follows that $\{\!\{J,J\}\!\} \subset \mathbb{Z}[\pi] \otimes J + J \otimes \mathbb{Z}[\pi]$. Therefore, the composition of $\{\!\{-,-\}\!\}$ with $\varpi \otimes q$ induces a $\mathbb{Z}$-linear map

$$\{\!\{-,-\}\!\}_J : J/J^2 \otimes J/J^2 \longrightarrow \mathbb{Z}[F] \otimes J/J^2.$$

We now take a, b, c in A and let $\underline{a} := [a-1], \underline{b} := [b-1], \underline{c} := [c-1]$ in J/J^2. Besides, the corresponding elements $[a], [b], [c]$ in $\mathbb{A}$ are simply denoted by a, b, c, respectively. Using the "skew-symmetry" (A.4) and its consequence (A.10), we apply $\varpi \otimes q$ to (A.32) to get the following identity in $\mathbb{Z}[F] \otimes J/J^2$:

$$-\overline{\Big\langle \{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell'}, a \Big\rangle}\, \{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell''} \otimes \{\!\{\underline{b},\underline{c}\}\!\}_J^{r} - \{\!\{\underline{b}, \eta_J(\underline{a},\underline{c})\}\!\}_J + \{\!\{\underline{b},\underline{a}\}\!\}_J^{\ell} \otimes \eta_J(\{\!\{\underline{b},\underline{a}\}\!\}_J^{r}, \underline{c}) \; = \; 0.$$

Note that the first term in this identity is

$$\begin{aligned} \overline{\Big\langle \{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell'}, a \Big\rangle}\, \{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell''} \otimes \{\!\{\underline{b},\underline{c}\}\!\}_J^{r} \;\; &= \;\; \overline{\Big\langle \overline{\{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell''}}\, \{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell'}, a \Big\rangle} \otimes \{\!\{\underline{b},\underline{c}\}\!\}_J^{r} \\ &\quad -\varepsilon(\{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell'})\overline{\Big\langle \overline{\{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell''}}, a \Big\rangle} \otimes \{\!\{\underline{b},\underline{c}\}\!\}_J^{r} \\ &= \;\; -\overline{\Big\langle \overline{\{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell}}, a \Big\rangle} \otimes \{\!\{\underline{b},\underline{c}\}\!\}_J^{r}. \end{aligned}$$

Therefore, we get

$$\text{(A.33)} \quad \overline{\Big\langle \overline{\{\!\{\underline{b},\underline{c}\}\!\}_J^{\ell}}, a \Big\rangle} \otimes \{\!\{\underline{b},\underline{c}\}\!\}_J^{r} - \{\!\{\underline{b}, \eta_J(\underline{a},\underline{c})\}\!\}_J + \{\!\{\underline{b},\underline{a}\}\!\}_J^{\ell} \otimes \eta_J(\{\!\{\underline{b},\underline{a}\}\!\}_J^{r}, \underline{c}) \; = \; 0.$$

It also follows from the definitions that

$$\text{(A.34)} \qquad \forall u,v \in \mathsf{A}, \quad \{\!\{[u-1],[v-1]\}\!\}_J = \overline{\Psi(u,v)^{\ell'}} \otimes \gamma\big(\Psi(u,v)^{\ell''} \otimes \Psi(u,v)^{r}\big),$$

which, using (A.8) and (A.10), implies the following more general formula:

$$\text{(A.35)}\ \forall u,v \in \mathsf{A}, \forall x \in \pi, \qquad \begin{aligned} &\{\!\{[u-1],[x(v-1)]\}\!\}_J \\ = \;\; &\varpi(x)\overline{\Psi(u,v)^{\ell'}} \otimes \gamma\big(\Psi(u,v)^{\ell''} \otimes \Psi(u,v)^{r}\big), \end{aligned}$$

$$-\Theta(\varpi(x),u)^r \otimes \gamma\left(\Theta(\varpi(x),u)^\ell \otimes (v-1)\right)$$

Then, using (A.34) and (A.35), we can rewrite the identity (A.33) as follows:

$$\begin{aligned}
&\overline{\langle\Psi(b,c)^{\ell'},a\rangle} \otimes \Psi(b,c)^{\ell''} \otimes \Psi(b,c)^r\\
-\Psi(a,c)^\ell\,&\overline{\Psi(b,\Psi(a,c)^r)^{\ell'}} \otimes \Psi(b,\Psi(a,c)^r)^{\ell''} \otimes \Psi(b,\Psi(a,c)^r)^r\\
&+\Theta(\Psi(a,c)^\ell,b)^r \otimes \Theta(\Psi(a,c)^\ell,b)^l \otimes \Psi(a,c)^r\\
+\overline{\Psi(b,a)^{\ell'}} \otimes \Psi(b,a)^{\ell''}&\Psi(\Psi(b,a)^r,c)^\ell \otimes \Psi(\Psi(b,a)^r,c)^r \quad = \quad 0.
\end{aligned}$$

From this identity, we can derive (A.30) and (A.31) by applying the automorphisms $(u\otimes v\otimes w \mapsto \overline{u'}\otimes u''v\otimes w)$ and $(u\otimes v\otimes w \mapsto uv'\otimes v''\otimes w)$ of $\mathbb{Z}[F]^{\otimes 2}\otimes \mathbb{A}$, respectively. □

Remark A.6. Let (α,β) be a basis of π of type (5.4), and set $a_i = [\alpha_i] \in \mathbb{A}$. It follows from (A.5) that $\Psi(a_i,a_j) = \delta_{i,j}\otimes a_i$ for any $i,j\in\{1,\dots,g\}$, and the values of $\Psi({}^x a_i, {}^y a_j)$ for arbitrary $x,y\in F$ are computed from (A.27) and (A.28).

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