An algebraic approach to multiple q-zeta values

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Contents

1 Introduction

1.1 Summary and results. In this thesis, we give several results on algebraic aspects of multiple q-zeta values. We assume that the reader is familiar with multiple zeta values; an overview is given in Appendix B. To integers $s_1 \geq 1,\ s_2, \dots, s_l \geq 0$ and polynomials $R_1 \in t\mathbb{Q}[t],\ R_2, \dots, R_l \in \mathbb{Q}[t]$, associate the generic multiple q-zeta value

$$\zeta_q(s_1, ..., s_l; R_1, ..., R_l) = \sum_{n_1 > \cdots > n_l > 0} \frac{R_1(q^{n_1})}{(1-q^{n_1})^{s_1}} \cdots \frac{R_l(q^{n_l})}{(1-q^{n_l})^{s_l}} \in \mathbb{Q}[[q]].$$

Generic multiple q-zeta values are q-analogs of multiple zeta values (Proposition 2.2). Moreover, the product of any two generic multiple q-zeta values is a $\mathbb{Q}$-linear combination of generic multiple q-zeta values.

Definition 1.1. The algebra of multiple q-zeta values is the subalgebra of $\mathbb{Q}[[q]]$ given by

$$\mathcal{Z}_q = \operatorname{span}_{\mathbb{Q}}\{\zeta_q(s_1, ..., s_l; R_1, ..., R_l) \mid l \geq 0, s_1 \geq 1,\ s_2, ..., s_l \geq 0, \deg(R_j) \leq s_j\},$$

where we set $\zeta_q(\emptyset; \emptyset) = 1$.

The additional requirement on the degree of the polynomials is justified by the relation of $\mathcal{Z}_q$ and polynomial functions on partitions ([BI22], Proposition 2.8). In particular, one obtains nice spanning sets of $\mathcal{Z}_q$ invariant under some involution.

The space $\mathcal{Z}_q$ is central to this thesis. H. Bachmann and U. Kühn proposed several conjectures about the algebraic structure of $\mathcal{Z}_q$ in [BK20], in particular, they conjectured that $\mathcal{Z}_q$ is a free polynomial algebra. In this work, we will give an algebraic approach to these conjectures. A model of multiple q-zeta values is given by a particular assumption on the polynomials R_i (usually these particular polynomials form a basis of $\mathbb{Q}[t]$). Various well-studied models of multiple q-zeta values are contained in $\mathcal{Z}_q$, an overview is given in [BK20] and [Br21]. The space $\mathcal{Z}_q$ also occurs in enumerative geometry. More precisely, A. Okounkov conjectured that certain generating series of Chern characters on Hilbert schemes of points are always contained in the space $\mathcal{Z}_q$ ([Ok14], [Qi18]).
Traditionally models of multiple q-zeta values focus on a q-analog of the shuffle product or the stuffle product obtained for multiple zeta values but do not combine them. So usually, it is difficult to describe a q-analog of the double shuffle relations. In rather recent articles on multiple q-zeta values by H. Bachmann ([Ba19]) and by K. Ebrahimi-Fard, D. Manchon, and J. Singer ([EMS16]) the focus changed to obtaining a product formula and some invariance under an involution, from which one easily derives a q-analog of the double shuffle relations. In joint work with H. Bachmann ([BB22]), we constructed the first model for multiple q-zeta values, which seems to satisfy a weight-graded product formula and invariance under some weight-homogeneous involution. Finally, the quasi-modular forms (with rational coefficients) expressed in their q-series expansion are contained in the algebra $\mathcal{Z}_q$, in the following, we will identify the algebra $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$ of the quasi-modular forms with rational coefficients with its image in $\mathcal{Z}_q$.

We introduce a spanning set of $\mathcal{Z}_q$ consisting of the balanced multiple q-zeta values $\zeta_q(s_1, \dots, s_l),\ s_1 \geq 1,\ s_2, \dots, s_l \geq 0$ (Definition 2.56). The classical Eisenstein series and their derivatives are particular examples of balanced multiple q-zeta values. One advantage of this model is that it gives an explicit description of a conjectural weight-grading on the algebra $\mathcal{Z}_q$, which extends the grading of the algebra $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$. Moreover, the balanced multiple q-zeta values satisfy a product formula, which can be seen as a balanced combination of the shuffle and stuffle product obtained for the multiple zeta values (cf (4.8.1)), and satisfy linear relations coming from a particular simple involution.

We study the algebraic structure of $\mathcal{Z}_q$ and its relation to the space $\mathcal{Z}$ of multiple zeta values (see Appendix B) with the help of the balanced multiple q-zeta values. Their relations can be described in terms of a graded Hopf algebra, this leads to the definition of the algebra $\mathcal{Z}_q^f$ of formal multiple q-zeta values (Definition 4.12). In particular, we have a surjective algebra morphism $\mathcal{Z}_q^f \to \mathcal{Z}_q$, which is expected to be an isomorphism. We will see that the algebra $\mathcal{Z}_q^f$ represents an affine scheme[1] BM (Theorem 4.18), which contains the affine group scheme DM introduced by G. Racinet in [Rac00] for multiple zeta values (Theorem 4.21). This leads to a surjective algebra morphism $\mathcal{Z}_q^f \to \mathcal{Z}^f$ (Corollary 4.22).

We introduce the corresponding linearized space $\mathfrak{bm}_0$ to BM_0, which contains the double shuffle Lie algebra $\mathfrak{dm}_0$ (Theorem 4.28). We will obtain a q-twisted Magnus Lie algebra $(\mathfrak{mq}, \{-,-\}_q)$ (Theorem 3.20), which can be seen as a generalization of the twisted Magnus Lie algebra $(\mathfrak{mt}, \{-,-\})$ ([Rac00, Chapter II, 2.2]). The space $\mathfrak{mq}$ contains the linearized space $\mathfrak{bm}_0$ and we conjecture that the q-Ihara bracket $\{-,-\}_q$ also preserves the space $\mathfrak{bm}_0$. In particular, there should be an injective Lie algebra morphism $(\mathfrak{dm}_0, \{-,-\}) \hookrightarrow (\mathfrak{bm}_0, \{-,-\}_q)$. Moreover, we expect that $\mathfrak{bm}_0$ is dual to the Lie coalgebra of indecomposables of $\mathcal{Z}_q^f / \left(\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)\right)$, where the elements $\zeta_q^f(k)$ for $k \geq 2$ even should be seen as a formal analog of the classical Eisenstein series of weight k. In particular, we expect a decomposition

$$\mathcal{Z}_q^f \simeq \widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z})) \otimes \mathcal{U}(\mathfrak{bm}_0)^\vee.$$

Finally, since we expect an isomorphism $\mathcal{Z}_q^f \simeq \mathcal{Z}_q$, this gives evidence for $\mathcal{Z}_q$ being a free polynomial algebra. A proof for the similar result for the algebra $\mathcal{Z}^f$ of formal multiple zeta values is one of the main results in the thesis of G. Racinet ([Rac00]) and he attributes this result to Ecalle.

Particular subsets of the balanced multiple q-zeta values $\zeta_q(s_1, \ldots, s_l)$ (Definition 2.56) or of the brackets $g(k_1, \ldots, k_d)$ (Definition 2.27) should give much smaller spanning sets of $\mathcal{Z}_q$. More precisely, Bachmann and Kühn ([BK20]) computed some evidence for the following equalities

$$\mathcal{Z}_q = \mathrm{span}_{\mathbb{Q}} \left\{\zeta_q(k_1, \ldots, k_d) \mid k_1, \ldots, k_d \geq 1\right\} = \mathrm{span}_{\mathbb{Q}} \left\{g(k_1, \ldots, k_d) \mid k_j \in \{1,2,3\}\right\}.$$

A result towards the first equality is given in Section 6. Some speculations that $\mathcal{Z}_q$ equals the latter space are given in the outlook.

1.2 The algebraic structure of $\mathcal{Z}_q$. The space $\mathcal{Z}_q$ is an algebra for the usual multiplication of power series (Proposition 2.4). In contrast to the algebra $\mathcal{Z}$ of multiple zeta values, where the multiple zeta values themselves can be used to obtain a nice description of the homogeneous subspaces and (conjecturally all) relations in $\mathcal{Z}$, there is not such a canonical choice for a spanning set of $\mathcal{Z}_q$. So we obtain different expressions of the product in $\mathcal{Z}_q$ for each choice of a spanning set. Typically, these product expressions can be described as quasi-shuffle products on some non-commutative algebras (as defined by M. Hoffman in [Hof00]). Moreover, a spanning set of $\mathcal{Z}_q$ usually satisfies a second set of relations defined by some involution. More explicitly, let $\mathcal{A}$ be a countable alphabet and $\mathbb{Q}\langle\mathcal{A}\rangle$ the free algebra over $\mathbb{Q}$ generated by the alphabet $\mathcal{A}$ (possibly with some restrictions for the first and last letter of each word). Denote by $\mathbf{1}$ the empty word. Then for any

[1] Inspired by the notation DM for "double mélange" ([Rac00]), we use BM for "balanced mélange"

commutative and associative product $\diamond$ on $\mathbb{Q}\mathcal{A}$, the corresponding quasi-shuffle product $*_\diamond$ on $\mathbb{Q}\langle\mathcal{A}\rangle$ is recursively defined by $\mathbf{1} *_\diamond w = w *_\diamond \mathbf{1} = w$ and

$$au *_\diamond bv = a(u *_\diamond bv) + b(au *_\diamond v) + (a \diamond b)(u *_\diamond v)$$

for all $u, v, w \in \mathbb{Q}\langle\mathcal{A}\rangle$ and $a, b \in \mathcal{A}$. An important example in this work is the balanced quasi-shuffle product $*_q$, which is defined on the non-commutative algebra $\mathbb{Q}\langle\mathcal{B}\rangle$ generated by the alphabet $\mathcal{B} = \{b_0, b_1, b_2, \ldots\}$ and corresponds to

$$b_i \diamond_q b_j = \begin{cases} b_{i+j} & \text{if } i, j \geq 1, \\ 0 & \text{else} \end{cases}. \tag{1.1.1}$$

Modulo words containing the letters b_i for $i \geq 2$ we obtain the well-known shuffle product (Definition B.13) and restricted to the letters b_i for $i \geq 1$ the product $*_q$ is given by the usual stuffle product (Definition B.17), therefore we call $*_q$ the balanced quasi-shuffle product.

For each spanning set of $\mathcal{Z}_q$ considered in this work (Definition 2.9, 2.27, 2.47, 2.56) there exists a quasi-shuffle product $*_\diamond$ and an involution ρ both defined on some (subspace of a) non-commutative algebra $\mathbb{Q}\langle\mathcal{A}\rangle$, such that there is a ρ-invariant, surjective algebra morphism

$$(\mathbb{Q}\langle\mathcal{A}\rangle, *_\diamond, \rho) \to (\mathcal{Z}_q, \cdot).$$

Denote

$$\mathbb{Q}\langle\mathcal{A}\rangle/\!\sim_\rho \; = \mathbb{Q}\langle\mathcal{A}\rangle \big/ \big(\rho(w) - w \mid w \in \mathbb{Q}\langle\mathcal{A}\rangle\big).$$

Generalizing [BK20], the following algebra isomorphisms are expected

$$\left(\mathbb{Q}\langle\mathcal{A}\rangle/\!\sim_\rho, *_\diamond\right) \simeq (\mathcal{Z}_q, \cdot). \tag{1.1.2}$$

For the precise formulation in terms of each spanning set, we refer to Conjectures 2.22, 2.35, 2.51, and 2.60.

We want to explicate the previously illustrated picture for the different spanning sets of $\mathcal{Z}_q$. First, consider the Schlesinger-Zudilin (SZ) multiple q-zeta values

$$\zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l) = \zeta_q(s_1, \ldots, s_l; t^{s_1}, \ldots, t^{s_l}) = \sum_{n_1 > \cdots > n_l > 0} \frac{q^{n_1 s_1}}{(1 - q^{n_1})^{s_1}} \cdots \frac{q^{n_l s_l}}{(1 - q^{n_l})^{s_l}},$$

where $s_1 \geq 1,\ s_2, \ldots, s_l \geq 0$. Let $\mathcal{B} = \{b_0, b_1, b_2, \ldots\}$ be an alphabet and denote by $\mathbb{Q}\langle\mathcal{B}\rangle^0$ the subalgebra of $\mathbb{Q}\langle\mathcal{B}\rangle$ generated by all words which do not start in b_0. Moreover, define the quasi-shuffle product $*_{\mathrm{SZ}}$ on $\mathbb{Q}\langle\mathcal{B}\rangle^0$ by $b_i \diamond_{\mathrm{SZ}} b_j = b_{i+j}$ and the involution $\tau : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q}\langle\mathcal{B}\rangle^0$ by $\tau(\mathbf{1}) = \mathbf{1}$ and

$$\tau(b_{k_1} b_0^{m_1} \ldots b_{k_d} b_0^{m_d}) = b_{m_d+1} b_0^{k_d-1} \ldots b_{m_1+1} b_0^{k_1-1}. \tag{1.1.3}$$

Due to J. Singer and Y. Takeyama (Theorem 2.13), there is a τ-invariant, surjective algebra morphism

$$\begin{aligned}(\mathbb{Q}\langle\mathcal{B}\rangle^0, *_{\mathrm{SZ}}, \tau) &\to (\mathcal{Z}_q, \cdot), \\ b_{s_1} \ldots b_{s_l} &\mapsto \zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l).\end{aligned}$$

Moreover, define for a SZ multiple q-zeta value $\zeta_q^{\mathrm{SZ}}(s_1,\dots,s_l)$ the weight as $s_1+\dots+s_l+|\{s_i\mid i=0\}|$ and the depth as $l-|\{s_i\mid i=0\}|$. This endows the algebra $\mathcal{Z}_q$ with two compatible filtrations.

Another well-studied spanning set of $\mathcal{Z}_q$ is given by the bi-brackets

$$g\binom{k_1,\dots,k_d}{m_1,\dots,m_d}=\frac{1}{(k_1-1)!\dots(k_d-1)!}\sum_{\substack{u_1>\dots>u_d>0\\ v_1,\dots,v_d>0}} u_1^{m_1}\dots u_d^{m_d}v_1^{k_1-1}\dots v_d^{k_d-1}q^{u_1v_1+\dots+u_dv_d},$$

where $k_1,\dots,k_d\geq 1,\ m_1,\dots,m_d\geq 0$. Consider the alphabet $\mathcal{Y}^{\mathrm{bi}}=\{y_{k,m}\mid k\geq 1,\ m\geq 0\}$ and let $\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle$ be the free non-commutative algebra generated by $\mathcal{Y}^{\mathrm{bi}}$. Then by the work of H. Bachmann (Theorem 2.32, 2.34), there is a swap invariant, surjective algebra morphism

$$\begin{aligned}(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle,*_{\mathrm{bb}},\mathrm{swap})&\to(\mathcal{Z}_q,\cdot),\\ y_{k_1,m_1}\cdots y_{k_d,m_d}&\mapsto g\binom{k_1,\dots,k_d}{m_1,\dots,m_d},\end{aligned}$$

where $*_{\mathrm{bb}}$ is defined in (2.31.1) and swap invariance is defined in (C.10).

The product $*_{\mathrm{SZ}}$ of the SZ multiple q-zeta values as well as the product $*_{\mathrm{bb}}$ of the bi-brackets are filtered by weight. We are interested in a spanning set of $\mathcal{Z}_q$, which satisfies a weight-graded product formula and is invariant under some homogeneous involution. In joint work with H. Bachmann ([BB22]), we obtained a construction of such a spanning set for $\mathcal{Z}_q$.

Theorem 1.2. *(2.46, 2.50) There is a swap invariant, surjective algebra morphism*

$$\begin{aligned}(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle,*,\mathrm{swap})&\to(\mathcal{Z}_q,\cdot),\\ y_{k_1,m_1}\cdots y_{k_d,m_d}&\mapsto G\binom{k_1,\dots,k_d}{m_1,\dots,m_d},\end{aligned}$$

where $G\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$ are the combinatorial bi-multiple Eisenstein series given in Definition 2.47 and $*$ is the quasi-shuffle product defined by $y_{k_1,m_1}\diamond y_{k_2,m_2}=y_{k_1+k_2,m_1+m_2}$.

For $k+m$ even, the combinatorial bi-Eisenstein series $G\binom{k}{m}$ equal the classical Eisenstein series and their derivatives. The algebra $(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle,*)$ is the associated weight-graded algebra to $(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle,*_{\mathrm{bb}})$, so the combinatorial multiple bi-Eisenstein series can be seen as a weight-graded version of the bi-brackets. In particular, it is expected that the combinatorial bi-multiple Eisenstein series endow the algebra $\mathcal{Z}_q$ with a weight-grading (Proposition 2.52).

Using the combinatorial multiple bi-Eisenstein series, we can define a spanning set of $\mathcal{Z}_q$, which can be seen as a weight-graded version of the SZ multiple q-zeta values.

Theorem 1.3. *(2.59) There is a τ-invariant, surjective algebra morphism*

$$\begin{aligned}(\mathbb{Q}\langle\mathcal{B}\rangle^0,*_q,\tau)&\to(\mathcal{Z}_q,\cdot),\\ b_{s_1}\dots b_{s_l}&\mapsto\zeta_q(s_1,\dots,s_l),\end{aligned}$$

where $\zeta_q(s_1,\dots,s_l)$ are the balanced multiple q-zeta values introduced in Definition 2.56 and $*_q$ is the balanced quasi-shuffle product given in (1.1.1).

The balanced multiple q-zeta values equip the algebra $\mathcal{Z}_q$ with the same conjectural weight-grading as the combinatorial bi-multiple Eisenstein series.

1.3 Formal multiple q-zeta values. Similar to the case of multiple zeta values (Definition B.22), we want to define a formal version $\mathcal{Z}_q^f$ of the algebra $\mathcal{Z}_q$. Since the balanced multiple q-zeta values $\zeta_q(s_1,\ldots,s_l)$ satisfy very explicit relations homogeneous in weight, this spanning set of $\mathcal{Z}_q$ is the natural choice from our point of view to determine the algebra $\mathcal{Z}_q^f$. More precisely, the algebra $\mathcal{Z}_q^f$ will be generated by formal symbols $\zeta_q^f(s_1,\ldots,s_l)$, for which we require to satisfy exactly the relations expected for the balanced multiple q-zeta values. According to (1.1.2), this means that the formal symbols $\zeta_q^f(s_1,\ldots,s_l)$ should multiply with respect to the balanced quasi-shuffle product $*_q$ and should be τ-invariant. To give such a definition of $\mathcal{Z}_q^f$ in terms of the quasi-shuffle algebra $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q)$, we have to introduce regularized multiple q-zeta values.

Theorem 1.4. *(4.11) There is a surjective algebra morphism*

$$\zeta_q^{\mathrm{reg}} : (\mathbb{Q}\langle\mathcal{B}\rangle, *_q) \to (\mathcal{Z}_q, \cdot),$$

which extends the map in Theorem 1.3 and satisfies $\zeta_q^{\mathrm{reg}}(b_0) = 0$.

Regularizing also the map τ similar to Theorem 4.11 does not give any new information and makes the defining conditions of the later introduced affine scheme BM (Definition 1.7) more complicated, thus we stick to considering τ as a map on $\mathbb{Q}\langle\mathcal{B}\rangle^0$. By the previous discussion, a natural definition of formal multiple q-zeta values is given by the following.

Definition 1.5. Define the algebra $\mathcal{Z}_q^f$ of formal multiple q-zeta values as

$$\mathcal{Z}_q^f = (\mathbb{Q}\langle\mathcal{B}\rangle, *_q)\big/_{\mathrm{Rel_q}},$$

where $\mathrm{Rel_q}$ is the ideal in $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q)$ generated by $\{b_0\} \cup \{w - \tau(w) \mid w \in \mathbb{Q}\langle\mathcal{B}\rangle^0\}$.

By construction, we have a surjective algebra morphism

$$\begin{aligned} \mathcal{Z}_q^f &\to \mathcal{Z}_q, \\ \zeta_q^f(w) &\mapsto \zeta_q^{\mathrm{reg}}(w). \end{aligned}$$

Reformulating (1.1.2), we expect that this map is an isomorphism of weight-graded algebras. The algebra $\mathcal{Z}_q^f$ is related to the algebra $\mathcal{Z}^f$ of formal multiple zeta values (Definition B.22), by Corollary 4.22 there is a surjective algebra morphism

$$p : \mathcal{Z}_q^f \twoheadrightarrow \mathcal{Z}^f.$$

In a slightly different context, the subspace of $\mathcal{Z}_q^f$ of depth ≤ 2 has been studied intensively in [BKM21]. The relations and realizations obtained there can be directly translated into the space $\mathcal{Z}_q^f$. Moreover, in [BIM] the algebra of formal multiple Eisenstein is studied, which is isomorphic to the algebra $\mathcal{Z}_q^f$

From the theory of quasi-shuffle algebras due to M. Hoffman ([Hof00],[HI17]) it is known that each quasi-shuffle algebra can be equipped with a Hopf algebra structure. More precisely, this means the following.

Proposition 1.6. *(4.2) The tuple* $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}})$ *is a commutative weight-graded Hopf algebra, where* Δ_{dec} *denotes the deconcatenation coproduct.*

For any commutative $\mathbb{Q}$-algebra R with unit, denote by $(R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q)$ the dual completed Hopf algebra to $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}})$ (Theorem 4.5). Then a non-commutative power series $\Phi \in R\langle\langle\mathcal{B}\rangle\rangle$ is grouplike for Δ_q, if and only if the coefficients of Φ multiply with respect to the balanced quasi-shuffle product $*_q$. Thus, similar to the case of multiple zeta values studied in [Rac00], we define the following.

Definition 1.7. For each commutative $\mathbb{Q}$-algebra R with unit, denote by $\mathsf{BM}(R)$ the set of all non-commutative power series Φ in $R\langle\langle\mathcal{B}\rangle\rangle$ satisfying

$$\begin{array}{lccc} \text{(i)} & (\Phi|b_0) & = & 0, \\ \text{(ii)} & \Delta_q(\Phi) & = & \Phi\hat{\otimes}\Phi, \\ \text{(iii)} & \tau(\Pi_0(\Phi)) & = & \Pi_0(\Phi), \end{array}$$

where Π_0 is the R-linear extension of the canonical projection $\mathbb{Q}\langle\mathcal{B}\rangle \to \mathbb{Q}\langle\mathcal{B}\rangle^0$.

For each $\lambda_1, \lambda_2, \lambda_3 \in R$, let $\mathsf{BM}_{(\lambda_1,\lambda_2,\lambda_3)}(R)$ be the subset of all $\Phi \in \mathsf{BM}(R)$ additionally satisfying

$$\text{(iv)} \quad (\Phi \mid b_2) = \lambda_1, \qquad (\Phi \mid b_4) = \lambda_2, \qquad (\Phi \mid b_6) = \lambda_3.$$

In the following, we will write $\mathsf{BM}_0(R) = \mathsf{BM}_{(0,0,0)}(R)$.

Also, the sets $\mathsf{BM}(R)$ and $\mathsf{DM}(R)$ (Definition B.24) are related, by Theorem 4.21 we have injective maps

$$\theta : \mathsf{DM}(R) \hookrightarrow \mathsf{BM}(R).$$

Theorem 1.8. *(4.18) The functor* $\mathsf{BM} : \mathbb{Q}\text{-}Alg \to Sets$ *is an affine scheme represented by the algebra* $\mathcal{Z}_q^f$ *of formal multiple q-zeta values.*
Similarly, the functor $\mathsf{BM}_0 : \mathbb{Q}\text{-}Alg \to Sets$ *is an affine scheme represented by the algebra*

$$\mathcal{Z}_q^f \big/ \left(\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)\right),$$

where $\left(\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)\right)$ *denotes the ideal in* $\mathcal{Z}_q^f$ *generated by* $\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)$.

As for DM_0 (Corollary B.31), we expect that BM_0 is a pro-unipotent affine group scheme.

1.4 Lie algebras and generators of $\mathcal{Z}_q$. By linearizing the defining equations of BM_0, we obtain a space consisting essentially of the algebra generators of $\mathcal{Z}_q^f$. We expect this space to be equipped with a Lie algebra structure.

Definition 1.9. Let $\mathfrak{bm}_0(R)$ be the $\mathbb{Q}$-vector space consisting of all non-commutative polynomials $\Psi \in R\langle\mathcal{B}\rangle$, which satisfy

$$\begin{array}{lcccl} \text{(i)} & (\Psi|b_0) & = & 0, & \\ \text{(ii)} & \Delta_q(\Psi) & = & \Psi \otimes \mathbf{1} + \mathbf{1} \otimes \Psi, & \\ \text{(iii)} & \tau(\Pi_0(\Psi)) & = & \Pi_0(\Psi), & \\ \text{(iv)} & (\Psi|b_k) & = & 0 & \text{for } k = 2,4,6. \end{array}$$

The space $\mathfrak{bm}_0(R)$ is graded by weight, denote by $\mathfrak{bm}_0(R)^{(w)}$ its homogeneous component of weight w. Set $\mathfrak{bm}_0 := \mathfrak{bm}_0(\mathbb{Q})$.

The space $\mathfrak{bm}_0$ should be seen as a generalization of the double shuffle Lie algebra $\mathfrak{dm}_0$ introduced in [Rac00], more precisely by Theorem 4.28 there is an explicit embedding of vector spaces

$$\theta : \mathfrak{dm}_0 \hookrightarrow \mathfrak{bm}_0.$$

After finding a suitable spanning set for $\mathcal{Z}_q$, namely the balanced multiple q-zeta values, and obtaining an explicit description of the space $\mathfrak{bm}_0$, the main task of this thesis was to equip $\mathfrak{bm}_0$ with a Lie algebra structure. A lot of explicit computations and tests (cf Subsection 4.7) as well as relating the space $\mathfrak{bm}_0$ to certain bimoulds (cf Subsection 5.4) led to an explicit formula for a conjectural Lie bracket on $\mathfrak{bm}_0$. Finally, we were able to prove the following.

Theorem 1.10. *(3.20, 3.21) There is a Lie algebra* $(\mathfrak{mq}, \{-,-\}_q)$ *with the following properties*

(i) The twisted Magnus Lie algebra $(\mathfrak{mt}, \{-,-\})$ *embeds into* $(\mathfrak{mq}, \{-,-\}_q)$.

(ii) The space $\mathfrak{bm}_0$ *is contained in* $\mathfrak{mq}$.

We call $(\mathfrak{mq}, \{-,-\}_q)$ the q-twisted Magnus Lie algebra and $\{-,-\}_q$ the q-Ihara bracket. The space $\mathfrak{bm}_0$ is conjecturally a Lie subalgebra of the q-twisted Magnus Lie algebra. More precisely, as for the double shuffle Lie algebra $\mathfrak{dm}_0$ (Theorem B.30, Corollary B.31), we expect the following for the space $\mathfrak{bm}_0$.

Conjecture 1.11.
(i) The space $\mathfrak{bm}_0$ *is a weight-graded Lie algebra equipped with the q-Ihara bracket* $\{-,-\}_q$.

(ii) The functor BM_0 *is a pro-unipotent affine group scheme with Lie algebra* $\widehat{\mathfrak{bm}_0}$.

(iii) For any commutative $\mathbb{Q}$*-algebra* R *with unit and all* $\lambda_1, \lambda_2, \lambda_3 \in R$*, the group* $\mathsf{BM}_0(R)$ *acts freely and transitively on* $\mathsf{BM}_{(\lambda_1,\lambda_2,\lambda_3)}(R)$*. We obtain an isomorphism of affine schemes*

$$\mathbb{A}^3 \times \widehat{\mathfrak{bm}_0} \xrightarrow{\sim} \mathsf{BM}.$$

Part (i) of the conjecture is checked[2] up to weight 9. Moreover, the associated depth-graded space of $\mathfrak{bm}_0$ embeds into a Lie algebra $(\mathfrak{lq}, \{-,-\}_q^D)$, which will be described below. The second and third part of Conjecture 1.11 should be a consequence of the first part, though this seems to require some more work. Similar to Ecalle's free generation theorem (Corollary B.32), we could deduce from Conjecture 1.11 the following.

Theorem 1.12. *(4.27) If Conjecture 1.11 holds, then we have an isomorphism of algebras*

$$\mathcal{Z}_q^f \simeq \widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z})) \otimes_{\mathbb{Q}} \mathcal{U}(\mathfrak{bm}_0)^\vee.$$

In particular, $\mathcal{Z}_q^f$ *would be a free polynomial algebra.*

A vague formulation of this conjecture is given in [BK20] based on their study of the Hilbert-Poincare series of these spaces.

We want to study the associated depth-graded space to $\mathfrak{bm}_0$.

Definition 1.13. Let $\mathfrak{lq}$ be the $\mathbb{Q}$-vector space given by all non-commutative polynomials $\Psi \in \mathbb{Q}\langle\mathcal{B}\rangle$ satisfying

$$\begin{array}{llcll} \text{(i)} & (\Psi|b_0) & = & 0, & \\ \text{(ii)} & \Delta_{ш}(\Psi) & = & \Psi\otimes\mathbf{1}+\mathbf{1}\otimes\Psi, & \\ \text{(iii)} & \tau(\Pi_0(\Psi)) & = & \Pi_0(\Psi), & \\ \text{(iv)} & (\Psi|b_kb_0^m) & = & 0 & k+m \text{ even}, \end{array}$$

where $\Delta_{ш}$ denotes the usual shuffle coproduct on $\mathbb{Q}\langle\mathcal{B}\rangle$ (Example A.62).

The weight- and depth-graded space $\mathfrak{lq}$ is indeed a Lie algebra.

Theorem 1.14. *(4.63 The space* $\mathfrak{lq}$ *equipped with the depth-graded q-Ihara bracket* $\{-,-\}_q^D$ *(Definition 4.62) is a bi-graded Lie algebra.*

[2] For example, one of the computed q-Ihara brackets consists of three terms with 147, 225 and 206 words and it is checked that it coincides with an element in $\mathfrak{bm}_0$ consisting of 205 words

Denote $\mathfrak{lb} = \mathrm{gr}_D\, \mathfrak{bm}_0$. Then by construction (Proposition 4.59), we have an embedding of vector spaces

$$\mathfrak{lb} \hookrightarrow \mathfrak{lq}.$$

But in contrast to the case of multiple zeta values, we do not expect this map to be surjective. Actually, there is an element in $\mathfrak{lq}$ of weight 8 and depth 2, which is not contained in $\mathfrak{lb}$ (Example 4.60). The Lie bracket $\{-,-\}_q^D$ defined for $\mathfrak{lq}$ is exactly the associated depth-graded to the q-Ihara bracket $\{-,-\}_q$, so by Conjecture 1.11 (i) we should have the following.

Conjecture 1.15. *The space* $\mathfrak{lb}$ *is a Lie subalgebra of* $(\mathfrak{lq}, \{-,-\}_q^D)$.

The Lie algebra $\mathfrak{lq}$ is related to the depth-graded double shuffle Lie algebra $\mathfrak{ls}$ obtained for multiple zeta values (Definition B.36), by Theorem 4.69 we have an injective Lie algebra morphism

$$\theta^D : (\mathfrak{ls}, \{-,-\}) \hookrightarrow (\mathfrak{lq}, \{-,-\}_q^D).$$

Since it is expected that $\mathfrak{ls} \simeq \mathrm{gr}_D\, \mathfrak{dm}_0$, the image of this embedding should lie in $\mathfrak{lb}$.

1.5 Lie algebras of bimoulds and $\mathcal{Z}_q$. We will briefly illustrate a second unpublished approach to Lie algebras related to $\mathcal{Z}_q$ in terms of bimoulds initiated by U. Kühn ([Kü19], [SK]), this is inspired by the work in [Ec11], [Sc15], and [IKZ06] for multiple zeta values. We assume that the reader is familiar with the theory of bimoulds, an introduction to moulds and bimoulds is given in Appendix C. For this approach, we consider the spanning set of $\mathcal{Z}_q$ given by the combinatorial bi-multiple Eisenstein series (Theorem 1.2). Let $\mathfrak{G} = (\mathfrak{G}_d)_{d\geq 0} \in \mathrm{GBARI}^{\mathrm{pow},\mathcal{Z}_q}$ be the bimould of generating series of the combinatorial bi-multiple Eisenstein series, i.e., $\mathfrak{G}_0 = 1$ and

$$\mathfrak{G}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d\end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}} G\begin{pmatrix} k_1,\dots,k_d \\ m_1,\dots,m_d\end{pmatrix} X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\dots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}, \qquad d\geq 1.$$

Let $\mathcal{Z}_q^{(w)}$ be the homogeneous subspace of $\mathcal{Z}_q$ spanned by all combinatorial bi-multiple Eisenstein series of weight w. Moreover, set $\overline{\mathcal{Z}}_q = \mathcal{Z}_q / \widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))\mathcal{Z}_q$ and denote by $\overline{\mathcal{Z}}_q^{(w)}$ the image of the homogeneous subspace $\mathcal{Z}_q^{(w)}$ in $\overline{\mathcal{Z}}_q$. Let $\mathcal{I}_q = \bigoplus_{w\geq 1} \overline{\mathcal{Z}}_q^{(w)}$, then

$$\mathcal{T}_q = \mathcal{I}_q / \mathcal{I}_q^2$$

is a weight-graded algebra and all products of multiple q-zeta values become trivial in $\mathcal{T}_q$.

Theorem 1.16. *(5.2) The projection of the bimould* $\mathfrak{G} \in \mathrm{GBARI}^{\mathrm{pow},\mathcal{Z}_q}$ *onto* $\mathrm{BARI}^{\mathrm{pow},\mathcal{T}_q}$ *is an element in*

$$\mathrm{BARI}^{\mathrm{pow},\mathcal{T}_q}_{\underline{\mathrm{il}},\mathrm{swap}} = \left\{ A \in \mathrm{BARI}^{\mathrm{pow},\mathcal{T}_q} \;\middle|\; \begin{array}{l} \cdot\ A \text{ is alternil}, \\ \cdot\ A \text{ is swap invariant}, \\ \cdot\ A_1\binom{X_1}{Y_1} \text{ is even} \end{array} \right\}.$$

There is a Lie bracket uri proposed by L. Schneps and used in [SK] (Definition 5.10), which preserves by construction the space of alternil bimoulds. Unfortunately, the definition involves poles, thus it is not clear whether the Lie bracket uri preserves the space of polynomial bimoulds. We obtained in this thesis a pre-Lie multiplication preuri (Definition 5.15), for which we can show that it preserves the space of polynomial bimoulds (Proposition 5.14) and for which we expect (Conjecture 5.16)

$$\mathrm{uri}(A,B) = \mathrm{preuri}(A,B) - \mathrm{preuri}(B,A), \qquad A,B \in \mathrm{BARI}^{\mathrm{pow}}\,.$$

Moreover, it is expected that the Lie bracket uri is compatible with swap invariance for alternil bimoulds.

Conjecture 1.17. *([SK]) The pair* $\left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}, \mathrm{uri}\right)$ *is a weight-graded Lie algebra.*

Next, consider the associated depth-graded space to $\mathcal{T}_q$,

$$\mathcal{M}_q = \bigoplus_{w,d\geq 1} \mathcal{M}_q^{(w,d)}, \qquad \mathcal{M}_q^{(w,d)} = \mathrm{gr}_D^{(d)}\,\mathcal{T}_q^{(w)}.$$

Theorem 1.18. *(5.22) The projection of the bimould* $\mathfrak{G} \in \mathrm{GBARI}^{\mathrm{pow},\mathcal{Z}_q}$ *onto* $\mathrm{BARI}^{\mathrm{pow},\mathcal{M}_q}$ *is contained in the space*

$$\mathrm{BARI}^{\mathrm{pow},\mathcal{M}_q}_{\underline{\mathrm{al}},\mathrm{swap}} = \left\{ A \in \mathrm{BARI}^{\mathrm{pow},\mathcal{M}_q} \;\middle|\; \begin{array}{l} \cdot\ A \textit{ is alternal,} \\ \cdot\ A \textit{ is swap invariant,} \\ \cdot\ A_1\binom{X_1}{Y_1} \textit{ is even} \end{array} \right\}.$$

The well-known ari bracket (Definition C.22) equips the space $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$ with a Lie algebra structure.

Theorem 1.19. *([SS20, Theorem 3.1, Proposition 3.4, 3.5]) The pair* $\left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}, \mathrm{ari}\right)$ *is a bi-graded Lie algebra.*

The associated depth-graded space to $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ properly embeds into the Lie algebra $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$ (Proposition 5.27). Moreover, the associated depth-graded to the uri bracket is exactly the ari bracket. Therefore, Conjecture 1.17 would imply that the space $\mathrm{gr}_D\,\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ is a Lie subalgebra of $\left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}, \mathrm{ari}\right)$.

The spaces $\mathfrak{bm}_0$ and $\mathfrak{lq}$ defined in terms of non-commutative polynomials (Definition 1.9, 1.13) are closely related to the spaces $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ and $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$ of bimoulds.

Theorem 1.20. *(i) (5.51) There is a vector space isomorphism*

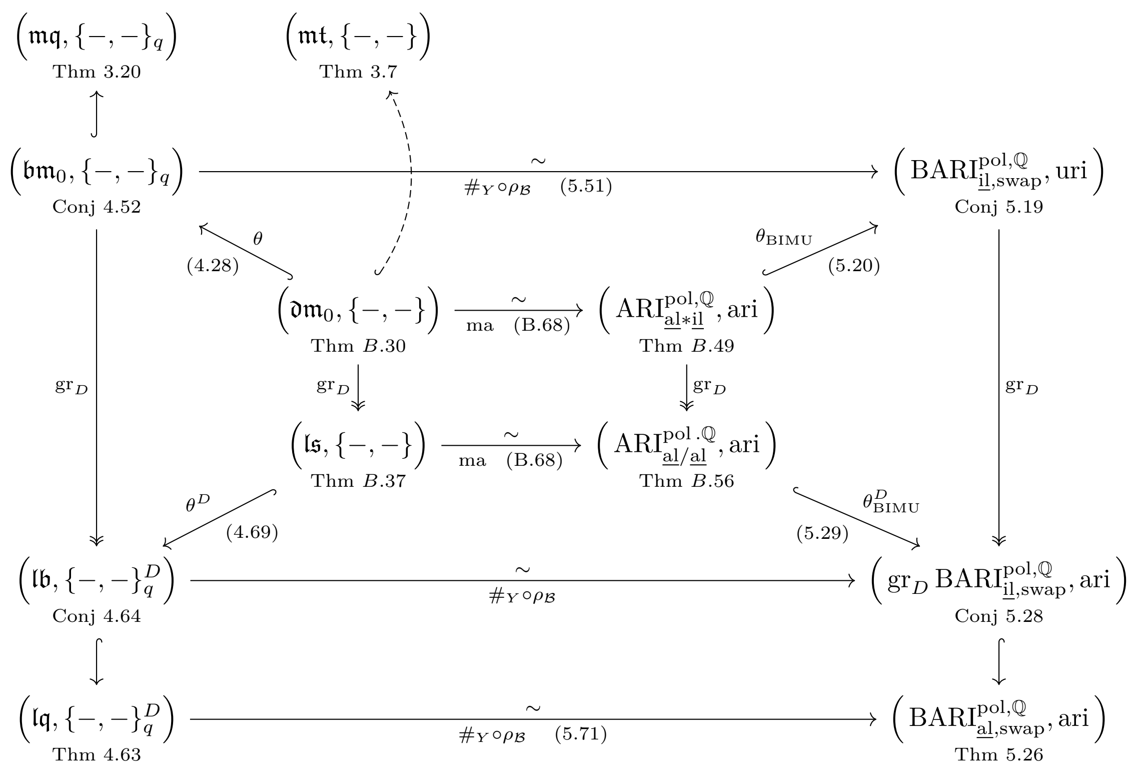
$$\#_Y \circ \rho_{\mathcal{B}} : \mathfrak{bm}_0 \xrightarrow{\sim} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\,.$$

(ii) (5.71) There is an isomorphism of bi-graded Lie algebras

$$\#_Y \circ \rho_{\mathcal{B}} : (\mathfrak{lq}, \{-,-\}_q^D) \xrightarrow{\sim} \left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}, \mathrm{ari}\right).$$

The q-Ihara bracket, which we expect to preserve the space $\mathfrak{bm}_0$, should correspond to the uri bracket, which is expected to preserve $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$, under the above isomorphism $\#_Y \circ \rho_{\mathcal{B}}$ (Theorem 5.52).

1.6 Overview on Lie algebras related to $\mathcal{Z}$ and $\mathcal{Z}_q$. Summarizing all our results on Lie algebras, we expect the following commutative diagram of Lie algebras related to multiple zeta values and multiple q-zeta values



The inner square summarizes the results of G. Racinet ([Rac00]) and J. Ecalle ([Ec11], [Ec02]) on Lie algebras related to multiple zeta values. The double shuffle Lie algebra $\mathfrak{dm}_0$ and its associated depth-graded $\mathfrak{ls}$ were obtained by G. Racinet in terms of non-commutative alphabets, the analog Lie algebra $\mathrm{ARI}^{\mathrm{pol}\,.\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ and $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ of moulds were discovered by J. Ecalle. G. Racinet ([Rac00]) and also L. Schneps ([Sc15]) related these two kinds of Lie algebras by the isomorphism ma.
The Lie algebras of bimoulds related to multiple q-zeta values were first studied by U. Kühn ([Kü19]). The Lie bracket uri was suggested by L. Schneps. It is a kind of an extension of the Lie bracket ari ([SK]). The conjectural Lie algebra $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ should be seen as a generalization of the Lie algebra $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ related to multiple zeta values. The associated depth-graded $\mathrm{gr}_D\,\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ embeds into the Lie algebra $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$.
As a main result of this thesis, we obtained an approach to Lie algebras related to multiple q-zeta values in terms of non-commutative alphabets similar to Racinet's approach to multiple zeta values. In particular, we obtained as a generalization of $\mathfrak{dm}_0$ and $\mathfrak{ls}$ the conjectural Lie algebra $\mathfrak{bm}_0$ and its associated depth-graded $\mathfrak{lb}$, which embeds into the Lie algebra $\mathfrak{lq}$. By relating these non-commutative spaces to the analog spaces of bimoulds via the map $\#_Y \circ \rho_{\mathcal{B}}$, we were able to discover the q-Ihara bracket $\{-,-\}_q$ and show that it equips the bigger space $\mathfrak{mq}$ indeed with a Lie algebra structure.

1.7 Lie algebras and dimension conjectures for $\mathcal{Z}_q$. As an analog of Zagier's dimension conjecture B.2 and the Broadhurst-Kreimer conjecture B.3 for multiple zeta values (or more precisely of Proposition B.7), there are dimension conjectures for the space $\mathcal{Z}_q$. Recall that a grading by weight $\mathcal{Z}_q = \bigoplus_{w\geq 0} \mathcal{Z}_q^{(w)}$ is expected, where $\mathcal{Z}_q^{(w)}$ denotes the subspace spanned by all balanced multiple q-zeta values or combinatorial bi-multiple

Eisenstein series of weight w.

Conjecture 1.21. *([BK20], Conjecture 1.3) (i) The dimensions of the homogeneous subspaces* $\mathcal{Z}_q^{(w)}$ *are given by*

$$\sum_{w\geq 0}\dim(\mathcal{Z}_q^{(w)})x^w = \frac{\widetilde{M}(x)}{1-D(x)O_1(x)+D(x)R(x)}$$
$$= \frac{1}{1-x-x^2-x^3+x^6+x^7+x^8+x^9},$$

where

$$D(x) = \frac{1}{1-x^2}, \qquad \widetilde{M}(x) = \sum_{k\geq 0}\dim\left(\widetilde{\mathcal{M}}_k(\mathrm{SL}_2(\mathbb{Z}))\right)x^k = \frac{1}{(1-x^2)(1-x^4)(1-x^6)},$$
$$O_1(x) = \frac{x}{1-x^2}, \qquad R(x) = \sum_{k\geq 4}\dim\left(\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))\oplus\mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z}))\right)x^k.$$

(ii) The dimensions of the homogeneous subspaces $\mathrm{gr}_D^{(d)}\,\mathcal{Z}_q^{(w)}$ *of the associated depth-graded space* $\mathrm{gr}_D\mathcal{Z}_q$ *are given by*

$$\sum_{w,d\geq 0}\dim\left(\mathrm{gr}_D^{(d)}\,\mathcal{Z}_q^{(w)}\right)x^w y^d = \frac{1+D(x)E_2(x)y+D(x)S(x)y^2}{1-a_1(x)y+a_2(x)y^2-a_3(x)y^3-a_4(x)y^4+a_5(x)y^5},$$

where

$$E_2(X) = \frac{x^2}{1-x^2}, \qquad S(x) = \sum_{k\geq 12}\dim(\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z})))x^k = \frac{x^{12}}{(1-x^4)(1-x^6)},$$

and

$$a_1(x) = D(x)O_1(x), \qquad a_2(x) = D(x)\sum_{k\geq 4}\dim(\mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z})))^2x^k,$$
$$a_3(x) = a_5(x) = D(x)xS(x), \qquad a_4(x) = D(x)\sum_{k\geq 12}\dim(\mathrm{S}_k(\mathrm{SL}_2(\mathbb{Z})))^2x^k.$$

Here $\widetilde{\mathcal{M}}_k(\mathrm{SL}_2(\mathbb{Z}))$, $\mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z}))$ *and* $\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ *denote the vector spaces of quasi-modular forms, modular forms, and cusp forms for* $\mathrm{SL}_2(\mathbb{Z})$ *of weight* k.

There is an efficient algorithm to compute the first 10.000 coefficients of an element in $\mathcal{Z}_q$. This algorithm was developed in [BK20] to provide Conjecture 1.21 and verify it up to weight 14 and all depths and up to weight 26 and depth 4.

Conjecture 1.22.
(i) The Lie algebra $\mathfrak{bm}_0$ *is equipped with a derivation, which increases the weight by* 2.
(ii) The Lie algebra $\mathfrak{bm}_0$ *has exactly one generator* $\xi\binom{k}{0}$ *in each odd weight* $k\geq 3$, *which is related to the double shuffle Lie algebra* $\mathfrak{dm}_0$. *Together with* $\xi\binom{1}{0} = b_1$ *and derivatives of these generators, one obtains a complete generating set for* $\mathfrak{bm}_0$. *The relations between the generators in weight* k *are counted by* $\dim\mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z}))\oplus\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$.
(iii) The Hilbert-Poincare series of the universal enveloping algebra of $\mathfrak{bm}_0$ *is*

$$H_{\mathcal{U}(\mathfrak{bm}_0)}(x) = \sum_{w\geq 0}\dim\mathcal{U}(\mathfrak{bm}_0)^{(w)}x^w = \frac{1}{1-D(x)O_1(x)+D(x)R(x)}.$$

Part (iii) follows from the first two parts of Conjecture 1.22. By Theorem 1.12 and the expected isomorphy $\mathcal{Z}_q^f \simeq \mathcal{Z}_q$, there should be also an isomorphism

$$\mathcal{Z}_q \simeq \widetilde{\mathcal{M}}(\mathrm{SL}_2(\mathbb{Z})) \otimes_{\mathbb{Q}} \mathcal{U}(\mathfrak{bm}_0)^{\vee}.$$

In particular, Conjecture 1.22 (iii) should be equivalent to the dimension conjecture 1.21 (i) for $\mathcal{Z}_q$.

For weight ≤ 13, we were able to check that Conjecture 1.22 (iii) holds. To obtain the dimensions of the spaces $\mathfrak{bm}_0^{(w)}$, we used another alphabet $\mathcal{V}$ satisfying (Corollary 4.33)

$$\mathfrak{bm}_0 \subset \mathrm{Lie}_{\mathbb{Q}}\langle \mathcal{V} \rangle.$$

Duval's algorithm ([BP94, Chapter 2]) allows to compute a Lyndon basis of $\mathrm{Lie}_{\mathbb{Q}}\langle \mathcal{V} \rangle^{(w)}$. Picking the (on $\mathbb{Q}\langle \mathcal{B} \rangle^0$) τ-invariant elements in the Lyndon basis then yields a basis of the space $\mathfrak{bm}_0^{(w)}$ (Theorem 4.39).

Similarly, there is an explicit expectation for the structure of the associated depth-graded Lie algebra $\mathfrak{lb}$ (Conjecture 1.15).

Conjecture 1.23.
(i) The Lie algebra $\mathfrak{lb}$ is generated by the depth 1 elements

$$\mathrm{gr}_D\, \xi \binom{k}{m} = \Big(-\mathrm{ad}(b_0) \Big)^m (b_k) + \Big(-\mathrm{ad}(b_0) \Big)^{k-1} (b_{m+1}), \qquad k \geq 1,\ m \geq 0,\ k+m \text{ odd},$$

and some elements in depth 4 introduced in Definition 5.37 in the spirit of Ecalle, which are counted by $\dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))^2$. They satisfy some relations in depths 2 and 5 related to modular forms.
(ii) The Hilbert-Poincare series of the universal enveloping algebra of $\mathfrak{lb}$ is

$$\begin{aligned} H_{\mathcal{U}(\mathfrak{lb})}(x,y) &= \sum_{w,d \geq 0} \dim \mathcal{U}(\mathfrak{lb})^{(w,d)} x^w y^d \\ &= \frac{1}{1 - a_1(x)y + a_2(x)y^2 - a_3(x)y^3 - a_4(x)y^4 + a_5(x)y^5}. \end{aligned}$$

By Theorem 1.12 and the expected isomorphy $\mathcal{Z}_q^f \simeq \mathcal{Z}_q$, there should be also a depth-graded algebra isomorphism

$$\mathrm{gr}_D\, {}^{\mathcal{Z}_q}\!\big/_{\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))\mathcal{Z}_q} \simeq \mathcal{U}(\mathfrak{lb})^{\vee}.$$

Therefore, Conjecture 1.23 (ii) should be equivalent to the dimension conjecture 1.21 (ii). Since there is a vector space isomorphism $\mathfrak{lb} \simeq \mathrm{gr}_D\, \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ (Theorem 1.20), one could check Conjecture 1.23 (ii) equivalently for the space $\mathrm{gr}_D\, \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$. This was done by U. Kühn ([Kü19]) up to weight 26 and depth 4. Moreover in Subsection 5.2, Conjecture 1.23 (i) is explained in detail in terms of the space $\mathrm{gr}_D\, \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$.

1.8 Outlook. The first steps towards discovering a Lie algebra, which is associated to multiple q-zeta values and generalizes the double shuffle Lie algebra $\mathfrak{dm}_0$, are presented in this work. This raises a lot of new problems and questions.

(i) The first point for future work is trying to find a proof that the space $\mathfrak{bm}_0$ equipped with the q-Ihara bracket $\{-,-\}_q$ is indeed a Lie algebra (Conjecture 1.11).

(ii) We expect a natural map $\exp : \widehat{\mathfrak{bm}_0} \to \mathsf{BM}_0$, which might be induced by the pre-Lie multiplication of the q-Ihara bracket (cf Theorem B.30). Applying Yoneda's Lemma to this exponential map would prove the algebra decomposition $\mathcal{Z}_q^f \simeq \widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z})) \otimes \mathcal{U}(\mathfrak{bm}_0)^\vee$ (Theorem 1.12).

(iii) The affine scheme BM_0 is expected to be a pro-unipotent affine group scheme with Lie algebra functor $\widehat{\mathfrak{bm}_0}$. Some partial results towards the group multiplication for BM_0 are given in Subsection 3.4.

(iv) Conjecture 1.22 (iii) predicts a connection between relations in $\mathfrak{bm}_0$ and modular forms, which is made explicit in the depth-graded case in terms of bimoulds (Theorem 5.34). There should be also an explicit way to connect the relations in $\mathfrak{bm}_0$ to (period polynomials of) modular forms.

(v) There should be a Lie algebra derivation on $\mathfrak{bm}_0$, which reduces to the explicit derivation on $\mathfrak{lq}$ (Proposition 4.68). Moreover, this derivation might be part of an $\mathfrak{sl}_2$-action, similar to the one obtained in [BIM] for a slightly different space.

(vi) The formula for the q-Ihara bracket is quite complicated. So it might be easier to make progress in the previously mentioned points by obtaining a notion of block degree and considering the associated block-graded space (cf Subsection B.5).

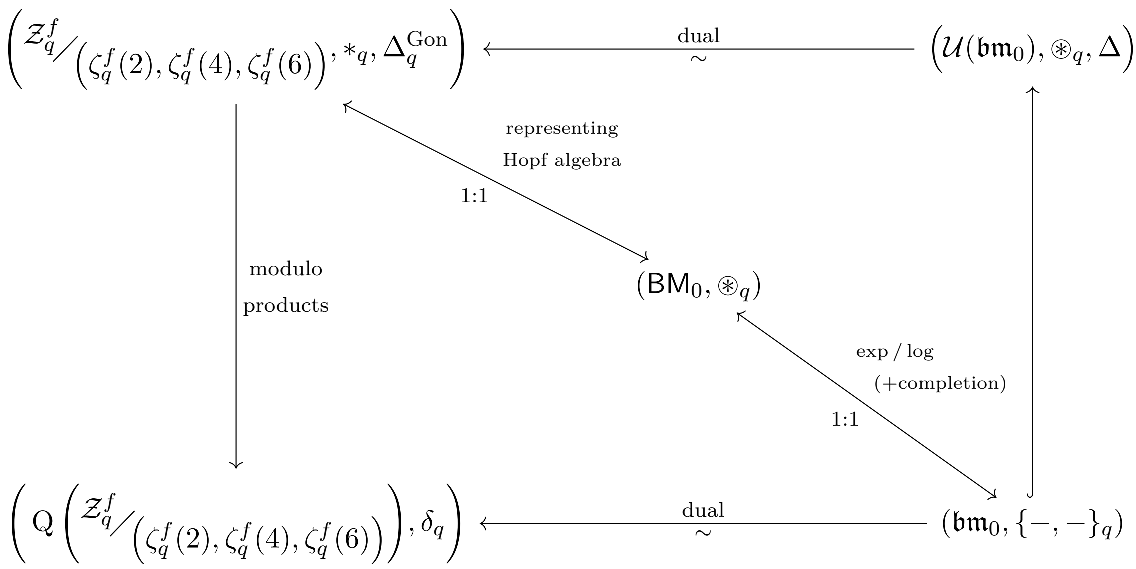
(vii) The q-Ihara bracket $\{-,-\}_q$ should determine a coproduct Δ_q^{Gon}, such that

$$\left(\mathcal{Z}_q^f \big/ \left(\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)\right), *_q, \Delta_q^{\mathrm{Gon}} \right)$$

becomes a weight-graded Hopf algebra. This might give a starting point to mimic Brown's techniques and find a small spanning set of $\mathcal{Z}_q$ (like the brackets with entries $1, 2, 3$).

(viii) There should be a motivic background for multiple q-zeta values, which allows obtaining upper bounds for the dimensions of the homogeneous subspaces of $\mathcal{Z}_q$.

In conclusion and similar to the situation of the formal multiple zeta values (B.35.1), we expect the following picture.



(1.23.1)

Here $\circledast_q$ denotes the dual product to the coproduct Δ_q^{Gon}, this might be hard to determine on the whole universal enveloping algebra $\mathcal{U}(\mathfrak{bm}_0)$. Moreover, the space of indecomposables $\mathrm{Q}\left(\mathcal{Z}_q^f \big/ \left(\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)\right)\right)$ is endowed with a Lie cobracket δ_q, which is induced by the coproduct Δ_q^{Gon} (Proposition A.42) and dual to the Lie bracket $\{-,-\}_q$ (Theorem A.43). The natural isomorphism $\exp : \widehat{\mathfrak{bm}_0} \to \mathsf{BM}_0$ should be obtained from Theorem A.95.

2 Graded, involutive models for $\mathcal{Z}_q$

We will consider the algebra of multiple q-zeta values $\mathcal{Z}_q$, which should be seen as a q-analog of the algebra of multiple zeta values. In contrast to the case of multiple zeta values, one has to restrict to certain spanning sets of $\mathcal{Z}_q$ to obtain nice descriptions of (conjectural all) relations in $\mathcal{Z}_q$. Actually, several models of multiple q-zeta values occur in the literature and most of them span the whole space $\mathcal{Z}_q$. An overview of these models is given in [BK20], [Br21], or [Zh20]. In particular, there are two well-known models for multiple q-zeta values, the Schlesinger-Zudilin multiple q-zeta values studied by K. Ebrahimi-Fard, D. Manchon, and J. Singer ([EMS16]) and the bi-brackets introduced by H. Bachmann ([Ba19]). Both of them satisfy a weight-filtered product formula and some homogeneous relations connected to an involution. So both models equip the algebra of multiple q-zeta values with a weight-filtered structure (and these structures coincide).
In analogy to the case of multiple zeta values, a weight-graded, involutive spanning set of $\mathcal{Z}_q$ seems to be a more canonical choice. There are two subsets of $\mathcal{Z}_q$ having these properties. The first spanning set is given by the combinatorial bi-multiple Eisenstein series ([BB22]), which are built from the bi-brackets and a rational solution to the extended double shuffle equations. They satisfy the associated weight-graded relations of the bi-brackets and conjecturally no other relations and thus they should induce a weight-grading on the algebra $\mathcal{Z}_q$. Unfortunately, the involutive relations among the combinatorial bi-multiple Eisenstein series become rather complicated in high depths and it is hard to write them down explicitly. This led us to another spanning set of $\mathcal{Z}_q$, the so-called balanced multiple q-zeta values, which should be seen as a weight-graded version of the Schlesinger-Zudilin multiple q-zeta values. Explicitly, we expect that they satisfy exactly the associated weight-graded relations of the Schlesinger-Zudilin multiple q-zeta values and hence also induce a weight-grading on $\mathcal{Z}_q$ (which is again the same as the one conjecturally induced by the combinatorial bi-multiple Eisenstein series). For the balanced multiple q-zeta values the product formula and also the involutive relations are quite easy to handle, therefore from our point of view, these objects provide the most natural choice for a spanning set of $\mathcal{Z}_q$. The balanced multiple q-zeta values are the main objects of this work, thus we will work out their structure in many details. In particular, we will use their algebraic structure to determine a conjectural Lie algebra consisting of non-commutative polynomials in Section 4.

2.1 The algebra of multiple q-zeta values

This subsection provides a short overview of the algebra of multiple q-zeta values, which was introduced in this form by H. Bachmann and U. Kühn ([BK20]).

Definition 2.1. To integers $s_1 \geq 1,\ s_2, \dots, s_l \geq 0$ and polynomials $R_1 \in t\mathbb{Q}[t],\ R_2, \dots, R_l \in \mathbb{Q}[t]$, we associate the generic multiple q-zeta value

$$\zeta_q(s_1, ..., s_l; R_1, ..., R_l) = \sum_{n_1 > \dots > n_l > 0} \frac{R_1(q^{n_1})}{(1-q^{n_1})^{s_1}} \cdots \frac{R_l(q^{n_l})}{(1-q^{n_l})^{s_l}}.$$

The assumptions $s_1 \geq 1$ and $R_1 \in t\mathbb{Q}[t]$ are necessary for convergence.

In general, a q-analog of some expression is a generalization involving the variable q, which returns the original expression by taking the limit $q \to 1$. E.g. a q-analog of some natural number $n \in \mathbb{N}$ is

$$\{n\}_q = \frac{1-q^n}{1-q} = 1 + q + \dots + q^{n-1},$$

since $\lim_{q\to 1}\{n\}_q = \underbrace{1+\cdots+1}_{n} = n.$

For all multi indices where the associated multiple zeta values are convergent, the generic multiple q-zeta values are (modified) q-analogs of multiple zeta values.

Proposition 2.2. *For $s_1 \geq 2,\ s_2,\dots,s_l \geq 1$ and $R_1 \in t\mathbb{Q}[t],\ R_2,\dots,R_l \in \mathbb{Q}[t]$, we have*

$$\lim_{q\to 1}(1-q)^{s_1+\cdots+s_l}\zeta_q(s_1,...,s_l;R_1,...,R_l) = R_1(1)\cdots R_l(1)\zeta(s_1,...,s_l).$$

Proof. This follows from the formal straight-forward calculation

$$\lim_{q\to 1}(1-q)^{s_1+\cdots+s_l}\zeta_q(s_1,...,s_l;R_1,...,R_l) = \lim_{q\to 1}\sum_{n_1>\cdots>n_l>0}\frac{R_1(q^{n_1})}{(\frac{1-q^{n_1}}{1-q})^{s_1}}\cdots\frac{R_l(q^{n_l})}{(\frac{1-q^{n_l}}{1-q})^{s_l}}$$
$$= \sum_{n_1>\cdots>n_l>0}\frac{R_1(1)}{n_1^{s_1}}\cdots\frac{R_l(1)}{n_l^{s_l}} = R_1(1)\cdots R_l(1)\zeta(s_1,...,s_l).$$

Convergence issues are justified with the same arguments as in [BK16, Proposition 6.4.]. □

Definition 2.3. Define the $\mathbb{Q}$-vector space spanned by all generic multiple q-zeta values

$$\mathcal{Z}_q = \operatorname{span}_{\mathbb{Q}}\{\zeta_q(s_1,...,s_l;R_1,...,R_l) \mid l \geq 0, s_1 \geq 1,\ s_2,...,s_l \geq 0, \deg(R_j) \leq s_j\},$$

where we set $\zeta_q(\emptyset;\emptyset) = 1$.

The additional assumption on the degree of the polynomials R_j will be justified by its relations to polynomial functions on partitions (Proposition 2.8). In particular, this definition allows to obtain nice spanning sets for $\mathcal{Z}_q$ invariant under some involution, those will be introduced in the next subsections.

For $\zeta_q(s_1;R_1), \zeta_q(s_2;R_2) \in \mathcal{Z}_q$, the usual power series multiplication reads

$$\zeta_q(s_1;R_1)\cdot\zeta_q(s_2;R_2) = \zeta_q(s_1,s_2;R_1,R_2) + \zeta_q(s_2,s_1;R_2,R_1) + \zeta_q(s_1+s_2;R_1R_2).$$

Since $\deg(R_1R_2) \leq s_1+s_2$, the product is also an element in $\mathcal{Z}_q$. Similar computations for arbitrary multi indices show the following.

Proposition 2.4. *The space $\mathcal{Z}_q$ is an associative, commutative algebra.* □

Thus, we will also refer to $\mathcal{Z}_q$ as the algebra of multiple q-zeta values.

Definition 2.5. We define the following subalgebras of $\mathcal{Z}_q$

$$\mathcal{Z}_q^\circ = \{\zeta_q(s_1,\dots,s_l;R_1,\dots,R_l) \in \mathcal{Z}_q \mid s_1,\dots,s_l \geq 1,\ R_1(t),\dots,R_l(t) \in t\mathbb{Q}[t]\},$$
$$\mathcal{Z}_{q,d} = \{\zeta_q(s_1,\dots,s_l;R_1,\dots,R_l) \in \mathcal{Z}_q \mid \deg(R_j) \leq s_j - d \text{ for } j=1,\dots,l\},$$
$$\mathcal{Z}_{q,d}^\circ = \mathcal{Z}_q^\circ \cap \mathcal{Z}_{q,d}.$$

A model for multiple q-zeta values is a spanning set of $\mathcal{Z}_q$ usually obtained by an explicit choice of the polynomials R_i. Various well-studied models can be identified with some of these subalgebras, an overview is given in [BK20], [Br21], and [Zh20]. Computational experiments lead to the following.

Conjecture 2.6. *([Ba19, Conjecture 4.3]) The following holds*

$$\mathcal{Z}_q = \mathcal{Z}_q^\circ.$$

It follows directly from the definition that the algebra $\mathcal{Z}_q$ is closed under the derivation $q\frac{\mathrm{d}}{\mathrm{d}q}$, which plays an important role in the theory of quasi-modular forms. Actually, this also holds for the space $\mathcal{Z}_q^\circ$.

Proposition 2.7. *([BK16, Theorem 1.7]) The pairs $(\mathcal{Z}_q, q\frac{\mathrm{d}}{\mathrm{d}q})$ and $(\mathcal{Z}_q^\circ, q\frac{\mathrm{d}}{\mathrm{d}q})$ are differential algebras, in particular,*

$$q\frac{\mathrm{d}}{\mathrm{d}q}(\mathcal{Z}_q) \subseteq \mathcal{Z}_q, \qquad q\frac{\mathrm{d}}{\mathrm{d}q}(\mathcal{Z}_q^\circ) \subseteq \mathcal{Z}_q^\circ.$$

□

There are explicit formulas expressing the derivation $q\frac{\mathrm{d}}{\mathrm{d}q}$ in terms of different models of multiple q-zeta values (e.g. in [Ba19, Proposition 4.2] and [Si15, Theorem 4.1]).

The restriction in the definition of $\mathcal{Z}_q$ to a special kind of generic multiple q-zeta values (Definition 2.3) can also be justified by relating $\mathcal{Z}_q$ to polynomial functions on partitions. In [BI22, cf (1.6)] it is shown that the space $\mathcal{Z}_q$ is exactly the image of the polynomial functions on partitions under the q-bracket.

Let $\lambda = (1^{m_1}2^{m_2}3^{m_3}\dots)$ be a partition of some natural number N of length d, i.e., the multiplicities $m_i \in \mathbb{Z}_{\geq 0}$ are nonzero only for finitely many indices $i_1, \dots, i_d$ and one has $\sum_{i\geq 1} m_i i = N$. A polynomial $f \in \mathbb{Q}[X_1, \dots, X_d, Y_1, \dots, Y_d]$ can be evaluated at the partition λ by

$$f(\lambda) = f(i_1, \dots, i_d, m_{i_1}, \dots, m_{i_d}).$$

E.g., for $\lambda = (1^2 2^0 3^1 4^0 5^0 \dots)$ and $f(X_1, X_2, Y_1, Y_2) = X_1 X_2 Y_1$ we obtain

$$f(\lambda) = f(1, 3, 2, 1) = 6.$$

Denote by $\mathcal{P}(N, d)$ the set of all partitions of N of length d.

Proposition 2.8. *([Br21, Theorem 1.3]) An element $F(q) \in \mathbb{Q}[[q]]$ lies in $\mathcal{Z}_q$, if and only if there exists a sequence $(f_d)_{d\geq 0} \in \bigoplus_{d\geq 0} \mathbb{Q}[X_1, \dots, X_d, Y_1, \dots, Y_d]$, such that*

$$F(q) = f_0 + \sum_{N\geq 1} \left(\sum_{d=1}^{N} \sum_{\lambda \in \mathcal{P}(N,d)} f_d(\lambda) \right) q^N.$$

□

2.2 Schlesinger-Zudilin multiple q-zeta values

We will study the Schlesinger-Zudilin multiple q-zeta values in their extended version, which were introduced by K. Ebrahimi-Fard, D. Manchon, and J. Singer ([EMS16]). They form a spanning set for $\mathcal{Z}_q$ and thus endow the algebra with a weight and depth filtration. Similar to the multiple zeta values their algebraic structure can be described in terms of two alphabets, an infinite one and a finite one.

Definition 2.9. To integers $s_1 \geq 1, s_2, \ldots, s_l \geq 0$, associate the Schlesinger-Zudilin (SZ) multiple q-zeta value

$$\zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l) = \sum_{n_1 > \cdots > n_l > 0} \frac{q^{n_1 s_1}}{(1-q^{n_1})^{s_1}} \cdots \frac{q^{n_l s_l}}{(1-q^{n_l})^{s_l}}.$$

For an index $(s_1, \ldots, s_l) \in \mathbb{Z}_{\geq 0}^l$, the weight and depth is given by

$$\begin{aligned} \mathrm{wt}(s_1, \ldots, s_l) &= s_1 + \cdots + s_l + \#\{i \mid s_i = 0\}, \\ \mathrm{dep}(s_1, \ldots, s_l) &= l - \#\{i \mid s_i = 0\}. \end{aligned}$$

We will also refer to these numbers as the weight and depth of $\zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l)$.

Theorem 2.10. *([BK20, p. 7]) The following equalities hold*

$$\begin{aligned} \mathcal{Z}_q &= \mathrm{span}_{\mathbb{Q}}\big\{\zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l) \mid l \geq 0, s_1 \geq 1,\ s_2, \ldots, s_l \geq 0\big\}, \\ \mathcal{Z}_q^{\circ} &= \mathrm{span}_{\mathbb{Q}}\big\{\zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l) \mid l \geq 0,\ s_1, \ldots, s_l \geq 1\big\}. \end{aligned}$$

Here we set $\zeta_q^{\mathrm{SZ}}(\emptyset) = 1$.

Proof. For all integers $s_1 \geq 1,\ s_2, \ldots, s_l \geq 0$ we have

$$\zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l) = \zeta_q(s_1, \ldots, s_l; t^{s_1}, \ldots, t^{s_l}) \in \mathcal{Z}_q$$

and thus we deduce for $s_1, \ldots, s_l \geq 1$ that

$$\zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l) \in \mathcal{Z}_q^{\circ}.$$

On the other hand, the elements

$$t^j(1-t)^{s-j}, \quad j = 1, \ldots, s,$$

form a basis of $\{R \in t\mathbb{Q}[t] \mid \deg(R) \leq s\}$. Thus for each polynomial $R \in t\mathbb{Q}[t]$ of degree $\leq s$, there exist elements $\alpha_j \in \mathbb{Q}$, such that

$$\frac{R(t)}{(1-t)^s} = \sum_{j=1}^{s} \alpha_j \frac{t^j}{(1-t)^j}.$$

So any element in $\mathcal{Z}_q^{\circ}$ is a linear combination of SZ multiple q-zeta values with entries ≥ 1. Similarly, the elements

$$t^j(1-t)^{s-j},\ j = 0, \ldots, s,$$

are a basis of $\{R \in \mathbb{Q}[t] \mid \deg(R) \leq s\}$, so every element in $\mathcal{Z}_q$ is a linear combination of SZ multiple q-zeta values $\zeta_q^{\mathrm{SZ}}(s_1, \ldots, s_l)$ with $s_1 \geq 1,\ s_2, \ldots, s_l \geq 0$. □

By Theorem 2.10, the notions of weight and depth for SZ multiple q-zeta values endow the space $\mathcal{Z}_q$ with compatible ascending (vector space) filtrations

$$\begin{aligned}\mathrm{Fil}_W^{(w)}(\mathcal{Z}_q) &= \mathrm{span}_{\mathbb{Q}}\{\zeta_q^{\mathrm{SZ}}(s_1,\dots,s_l) \mid \mathrm{wt}(s_1,\dots,s_l) \le w\}, \\ \mathrm{Fil}_D^{(d)}(\mathcal{Z}_q) &= \mathrm{span}_{\mathbb{Q}}\{\zeta_q^{\mathrm{SZ}}(s_1,\dots,s_l) \mid \mathrm{dep}(s_1,\dots,s_l) \le d\}.\end{aligned} \tag{2.10.1}$$

The usual power series multiplication in $\mathcal{Z}_q$ can be expressed in terms of the SZ multiple q-zeta values, we will refer to this expression as the SZ stuffle product. To describe this explicitly, we introduce the following quasi-shuffle algebra (cf Subsection A.3).

Definition 2.11. Consider the alphabet $\mathcal{B} = \{b_0, b_1, b_2, \dots\}$ and let $\mathbb{Q}\langle\mathcal{B}\rangle$ be the free non-commutative algebra over $\mathcal{B}$. Moreover, denote by $\mathbf{1}$ the empty word.
Define the SZ stuffle product $*_{\mathrm{SZ}}$ to be the quasi-shuffle product on $\mathbb{Q}\langle\mathcal{B}\rangle$ corresponding to

$$b_i \diamond_{\mathrm{SZ}} b_j = b_{i+j}, \quad b_i, b_j \in \mathcal{B}.$$

For all $s_1,\dots,s_l \ge 0$, the weight and depth of the word $b_{s_1}\dots b_{s_l}$ is defined as

$$\begin{aligned}\mathrm{wt}(b_{s_1}\dots b_{s_l}) &= s_1 + \dots + s_l + \#\{i \mid s_i = 0\}, \\ \mathrm{dep}(b_{s_1}\dots b_{s_l}) &= l - \#\{i \mid s_i = 0\}.\end{aligned}$$

Then the pair $(\mathbb{Q}\langle\mathcal{B}\rangle, *_{\mathrm{SZ}})$ is a bi-filtered algebra with respect to weight and depth.

Definition 2.12. Let $\mathbb{Q}\langle\mathcal{B}\rangle^0$ be the subspace of $\mathbb{Q}\langle\mathcal{B}\rangle$ generated by all words, which do not start in b_0. Define the involution $\tau : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q}\langle\mathcal{B}\rangle^0$ by $\tau(\mathbf{1}) = \mathbf{1}$ and

$$\tau(b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}) = b_{m_d+1} b_0^{k_d-1} \dots b_{m_1+1} b_0^{k_1-1}$$

for all $k_1,\dots,k_d \ge 1$, $m_1,\dots,m_d \ge 0$.

The combinatorics of infinite nested sums imply that the SZ multiple q-zeta values multiply with respect to the SZ stuffle product $*_{\mathrm{SZ}}$. Even more, the following holds.

Theorem 2.13. *(i) ([Si15, Theorem 3.3]) There is a surjective algebra morphism*

$$\begin{aligned}\zeta_q^{\mathrm{SZ}} : (\mathbb{Q}\langle\mathcal{B}\rangle^0, *_{\mathrm{SZ}}) &\to (\mathcal{Z}_q, \cdot), \\ b_{s_1}\dots b_{s_l} &\mapsto \zeta_q^{\mathrm{SZ}}(s_1,\dots,s_l),\end{aligned}$$

which is compatible with the weight and depth filtrations.

(ii) ([Ta13, Theorem 4]) The morphism ζ_q^{SZ} is τ-invariant, i.e., one has for all integers $k_1,\dots,k_d \ge 1,\ m_1,\dots,m_d \ge 0$

$$\zeta_q^{\mathrm{SZ}}(k_1, \{0\}^{m_1}, \dots, k_d, \{0\}^{m_d}) = \zeta_q^{\mathrm{SZ}}(m_d+1, \{0\}^{k_d-1}, \dots, m_1+1, \{0\}^{k_1-1}).$$

□

The SZ stuffle product in Theorem 2.13 (i) is a q-analog of the usual stuffle product. Assuming $s_1 \ge 2,\ s_2,\dots,s_l \ge 1$ and applying the limit $q \to 1$ (after multiplying with a suitable power of $(1-q)$), one obtains the stuffle product formula of multiple zeta values (Proposition B.20).

Remark 2.14. The τ-invariance of the SZ multiple q-zeta values is quite similar to the duality of Zudilin's multiple q-zeta brackets ([Zu15, Proposition 4]).

Example 2.15. In depth 2, the SZ stuffle product reads

$$\begin{aligned}\zeta_q^{\mathrm{SZ}}(k_1,\{0\}^{m_1})\zeta_q^{\mathrm{SZ}}(k_2,\{0\}^{m_2}) = & \sum_{j=0}^{m}\Bigg(\sum_{i=0}^{m-j}\binom{m_2+1}{i}\binom{m-j-i}{m_2}\zeta_q^{\mathrm{SZ}}(k_1,\{0\}^j,k_2,\{0\}^{m-j-i}) \\ & + \sum_{i=0}^{m-j}\binom{m_1+1}{i}\binom{m-j-i}{m_1}\zeta_q^{\mathrm{SZ}}(k_2,\{0\}^j,k_1,\{0\}^{m-j-i}) \\ & + \binom{m_1}{j}\binom{m-j}{m_1}\zeta_q^{\mathrm{SZ}}(k_1+k_2,\{0\}^{m-j})\Bigg),\end{aligned}$$

where $k_1, k_2 \geq 1$ and $m_1, m_2 \geq 0,\ m = m_1 + m_2$.

An immediate consequence of Theorem 2.13 (i) is the compatibility of the product in $\mathcal{Z}_q$ with the weight and depth filtrations.

Corollary 2.16. *The notions of weight and depth for SZ multiple q-zeta values define two algebra filtrations on $\mathcal{Z}_q$. In particular,*

$$\mathrm{Fil}_D^{(d_1)}(\mathcal{Z}_q)\,\mathrm{Fil}_D^{(d_2)}(\mathcal{Z}_q) \subset \mathrm{Fil}_D^{(d_1+d_2)}(\mathcal{Z}_q), \qquad \mathrm{Fil}_W^{(w_1)}(\mathcal{Z}_q)\,\mathrm{Fil}_W^{(w_2)}(\mathcal{Z}_q) \subset \mathrm{Fil}_W^{(w_1+w_2)}(\mathcal{Z}_q).$$

J. Singer introduced in [Si15] a second finite alphabet to describe the algebraic structure of SZ multiple q-zeta values. This can be viewed as an analog of the finite alphabet $\mathcal{X}$ introduced for multiple zeta values (Definition B.13).

Definition 2.17. Let $\mathbb{Q}\langle p, y\rangle$ be the free algebra over $\mathbb{Q}$ generated by the alphabet $\{p, y\}$ and denote by $\mathbf{1}$ the empty word. Define the SZ shuffle product $ш_{\mathrm{SZ}}$ on $\mathbb{Q}\langle p, y\rangle$ recursively by $\mathbf{1} ш_{\mathrm{SZ}} w = w ш_{\mathrm{SZ}} \mathbf{1} = w$ and

$$\begin{aligned}(yu) ш_{\mathrm{SZ}} v = u ш_{\mathrm{SZ}} (yv) &= y(u ш_{\mathrm{SZ}} v), \\ (pu) ш_{\mathrm{SZ}} (pv) &= p(u ш_{\mathrm{SZ}} pv + pu ш_{\mathrm{SZ}} v + u ш_{\mathrm{SZ}} v)\end{aligned}$$

for all $u, v, w \in \mathbb{Q}\langle p, y\rangle$. Though we call this product the SZ shuffle product, it is not a quasi-shuffle product in the sense of Definition A.52. Moreover, denote by $\mathbb{Q}\langle p, y\rangle^0$ the subspace of $\mathbb{Q}\langle p, y\rangle$ spanned by all words starting in p and ending in y, so

$$\mathbb{Q}\langle p, y\rangle^0 = \mathbb{Q}\mathbf{1} + p\mathbb{Q}\langle p, y\rangle y.$$

Expressing the SZ multiple q-zeta values via iterated Rota-Baxter operators leads to

Proposition 2.18. *([Si15, Theorem 3.2.]) The map*

$$\begin{aligned}(\mathbb{Q}\langle p, y\rangle^0, ш_{\mathrm{SZ}}) &\to (\mathcal{Z}_q, \cdot), \\ p^{s_1}y\ldots p^{s_l}y &\mapsto \zeta_q^{\mathrm{SZ}}(s_1,\ldots,s_l)\end{aligned}$$

is a surjective algebra morphism. □

The SZ shuffle product in Proposition 2.18 can be seen as a q-analog of the shuffle product. Whenever $s_1 \geq 2,\ s_2,\ldots,s_l \geq 1$, then taking the limit $q \to 1$ (after multiplying with some power of $(1-q)$) yields the shuffle product formula for multiple zeta values (Proposition B.16).

Example 2.19. In depth 2, the SZ shuffle product is given by

$$\zeta_q^{\mathrm{SZ}}(k_1,\{0\}^{m_1})\zeta_q^{\mathrm{SZ}}(k_2,\{0\}^{m_2}) = \sum_{j=1}^{k-1}\Bigg(\sum_{i=0}^{k-1-j}\binom{j-1}{k_1-1}\binom{k_1}{i}\zeta_q^{\mathrm{SZ}}(j,\{0\}^{m_1},k-j-i,\{0\}^{m_2}) \\ + \sum_{i=0}^{k-1-j}\binom{j-1}{k_2-1}\binom{k_2}{i}\zeta_q^{\mathrm{SZ}}(j,\{0\}^{m_2},k-j-i,\{0\}^{m_1}) \\ + \binom{j-1}{k_1-1}\binom{k_1-1}{j-k_2}\zeta_q^{\mathrm{SZ}}(j,\{0\}^{m_1+m_2+1})\Bigg),$$

where $k_1,k_2\geq 1,\ k=k_1+k_2$ and $m_1,m_2\geq 0$.

The involution τ (Definition 2.12) can be also defined on the algebra $\mathbb{Q}\langle p,y\rangle$.

Definition 2.20. Let τ be the anti-automorphism on $\mathbb{Q}\langle p,y\rangle$ given by $\tau(\mathbf{1})=\mathbf{1}$ and $\tau(p)=y$, $\tau(y)=p$, i.e., one has for all $k_1,\dots,k_d\geq 1,\ m_0,\dots,m_d\geq 0$

$$\tau(y^{m_0}p^{k_1}y^{m_1}\dots p^{k_d}y^{m_d}) = p^{m_d}y^{k_d}\dots p^{m_1}y^{k_1}p^{m_0}.$$

The involution τ preserves the subalgebra $\mathbb{Q}\langle p,y\rangle^0$. Moreover, τ relates the SZ stuffle product $*_{\mathrm{SZ}}$ and the SZ shuffle product $⧢_{\mathrm{SZ}}$. To describe this relation, consider the canonical embedding

$$i:\mathbb{Q}\langle\mathcal{B}\rangle \hookrightarrow \mathbb{Q}\langle p,y\rangle, \\ b_{s_1}\dots b_{s_l}\mapsto p^{s_1}y\dots p^{s_l}y. \tag{2.20.1}$$

Theorem 2.21. *([EMS16, Theorem 5.4]) For all $u,v\in\mathbb{Q}\langle\mathcal{B}\rangle$, the following holds*

$$i(u*_{\mathrm{SZ}}v) = \tau\big(\tau\circ i(u)\,⧢_{\mathrm{SZ}}\,\tau\circ i(v)\big).$$

□

Since τ is an involution, one obtains an injective algebra morphism

$$\tau\circ i:(\mathbb{Q}\langle\mathcal{B}\rangle,*_{\mathrm{SZ}})\hookrightarrow(\mathbb{Q}\langle p,y\rangle,⧢_{\mathrm{SZ}}), \\ b_{s_1}\dots b_{s_l}\mapsto py^{s_l}\dots py^{s_1}.$$

This allows interpreting the restriction of $⧢_{\mathrm{SZ}}$ to $\mathrm{im}(\tau\circ i)=\mathbb{Q}\mathbf{1}+p\mathbb{Q}\langle p,y\rangle$ as a quasi-shuffle product.

Just as one expects the extended double shuffle relations among multiple zeta values to give all relations in $\mathcal{Z}$ (Conjecture B.9), the following is conjectured for the SZ multiple q-zeta values.

Conjecture 2.22. *([Ta13]) All relations in $\mathcal{Z}_q$ are a consequence of the SZ stuffle product and the τ-invariance (Theorem 2.13) of SZ multiple q-zeta values.*

Example 2.23. By applying the SZ stuffle product formula, we obtain

$$\zeta_q^{\mathrm{SZ}}(1)\zeta_q^{\mathrm{SZ}}(2) = \zeta_q^{\mathrm{SZ}}(1,2)+\zeta_q^{\mathrm{SZ}}(2,1)+\zeta_q^{\mathrm{SZ}}(3).$$

On the other hand, we can apply the SZ shuffle product formula. By Theorem 2.21, this means apply the τ-invariance to both factors, then multiply with respect to the SZ stuffle product formula and then again apply τ-invariance

$$\begin{aligned}\zeta_q^{\mathrm{SZ}}(1)\zeta_q^{\mathrm{SZ}}(2) &= \zeta_q^{\mathrm{SZ}}(1)\zeta_q^{\mathrm{SZ}}(1,0) \\ &= 2\zeta_q^{\mathrm{SZ}}(1,1,0)+\zeta_q^{\mathrm{SZ}}(1,0,1)+\zeta_q^{\mathrm{SZ}}(2,0)+\zeta_q^{\mathrm{SZ}}(1,1) \\ &= 2\zeta_q^{\mathrm{SZ}}(2,1)+\zeta_q^{\mathrm{SZ}}(1,2)+\zeta_q^{\mathrm{SZ}}(2,0)+\zeta_q^{\mathrm{SZ}}(1,1).\end{aligned}$$

Comparing both product expressions, we obtain

$$\zeta_q^{\mathrm{SZ}}(3)=\zeta_q^{\mathrm{SZ}}(2,1)+\zeta_q^{\mathrm{SZ}}(2,0)+\zeta_q^{\mathrm{SZ}}(1,1).$$

Multiplying by $(1-q)^3$ and applying the limit $q\to 1$, we recover Euler's well-known relation

$$\zeta(3)=\zeta(2,1).$$

We end this subsection by expressing the previously given algebraic relations of SZ multiple q-zeta values in terms of generating series. For each $d\geq 1$, define the generating series of the SZ multiple q-zeta values of depth d by

$$\mathfrak{s}\mathfrak{z}_d\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}=\sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}}\zeta_q^{\mathrm{SZ}}(k_1,\{0\}^{m_1},\dots,k_d,\{0\}^{m_d})X_1^{k_1-1}Y_1^{m_1}\dots X_d^{k_d-1}Y_d^{m_d} \tag{2.23.1}$$

and moreover set $\mathfrak{s}\mathfrak{z}_0=1$.

Lemma 2.24. *([Br21, Theorem 2.18]) For each $d\geq 1$, one has*

$$\begin{aligned}\mathfrak{s}\mathfrak{z}_d\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}&=\sum_{\substack{u_1>\dots>u_d>0\\ v_1,\dots,v_d>0}}\prod_{i=1}^d(1+X_i)^{v_i-1}(1+Y_i)^{u_i-u_{i+1}-1}q^{u_iv_i}\\ &=\sum_{u_1>\dots>u_d>0}\prod_{i=1}^d(1+Y_i)^{u_i-u_{i-1}-1}\frac{q^{u_i}}{1-(1+X_i)q^{u_i}},\end{aligned}$$

where $u_{d+1}:=0$. □

We reformulate the τ-invariance of the SZ multiple q-zeta values (Theorem 2.13 (ii)) in terms of these generating series.

Proposition 2.25. *For each $d\geq 1$, the generating series $\mathfrak{s}\mathfrak{z}_d$ is τ-invariant, i.e., one has*

$$\mathfrak{s}\mathfrak{z}_d\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}=\mathfrak{s}\mathfrak{z}_d\binom{Y_d,\dots,Y_1}{X_d,\dots,X_1}.$$

Proof. Using the τ-invariance of the SZ multiple q-zeta values (Theorem 2.13 (ii)), we compute for each $d\geq 1$

$$\begin{aligned}\mathfrak{s}\mathfrak{z}_d\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}&=\sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}}\zeta_q^{\mathrm{SZ}}(k_1,\{0\}^{m_1},\dots,k_d,\{0\}^{m_d})X_1^{k_1-1}Y_1^{m_1}\dots X_d^{k_d-1}Y_d^{m_d}\\ &=\sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}}\zeta_q^{\mathrm{SZ}}(m_d+1,\{0\}^{k_d-1},\dots,m_1+1,\{0\}^{k_1-1})X_1^{k_1-1}Y_1^{m_1}\dots X_d^{k_d-1}Y_d^{m_d}\\ &=\sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}}\zeta_q^{\mathrm{SZ}}(k_1,\{0\}^{m_1},\dots,k_d,\{0\}^{m_d})X_1^{m_1}Y_1^{k_d-1}\dots X_d^{m_1}Y_d^{k_1-1}\\ &=\mathfrak{s}\mathfrak{z}_d\binom{Y_d,\dots,Y_1}{X_d,\dots,X_1}.\end{aligned}$$

□

To describe the SZ stuffle product on the level of generating series, we have to consider generating series of words (Subsection A.4). In this case, define the generating series of words in $\mathbb{Q}\langle\mathcal{B}\rangle^0$ by $\rho_{\mathcal{B}}(\mathcal{W})_0 = \mathbf{1}$ and

$$\rho_{\mathcal{B}}(\mathcal{W})_d \binom{X_1, \dots, X_d}{Y_1, \dots, Y_d} = \sum_{\substack{k_1,\dots,k_d \geq 1 \\ m_1,\dots,m_d \geq 0}} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d} X_1^{k_1-1} Y_1^{m_1} \dots X_d^{k_d-1} Y_d^{m_d}, \quad d \geq 1.$$

Extend the SZ stuffle product defined on $\mathbb{Q}\langle\mathcal{B}\rangle^0$ as well as the SZ multiple q-zeta value map $\zeta_q^{\mathrm{SZ}} : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathcal{Z}_q$ (cf Theorem 2.13) by $\mathbb{Q}[[X_1, Y_1, X_2, Y_2, \dots]]$-linearity to the space $\mathbb{Q}\langle\mathcal{B}\rangle^0[[X_1, Y_1, X_2, Y_2, \dots]]$. Then, one obtains by definition for all $d \geq 1$

$$\zeta_q^{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})_d \binom{X_1, \dots, X_d}{Y_1, \dots, Y_d} \right) = \mathfrak{sz}_d \binom{X_1, \dots, X_d}{Y_1, \dots, Y_d}.$$

Since $\zeta_q^{\mathrm{SZ}} : (\mathbb{Q}\langle\mathcal{B}\rangle^0, *_{\mathrm{SZ}}) \to (\mathcal{Z}_q, \cdot)$ is an algebra morphism (Theorem 2.13 (i)), we immediately derive the following.

Proposition 2.26. *For all $0 < n < d$, we have*

$$\mathfrak{sz}_d \binom{X_1, \dots, X_n}{Y_1, \dots, Y_n} \mathfrak{sz}_{d-n} \binom{X_{n+1}, \dots, X_d}{Y_{n+1}, \dots, Y_d} = \zeta_q^{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})_n \binom{X_1, \dots, X_n}{Y_1, \dots, Y_n} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})_{d-n} \binom{X_{n+1}, \dots, X_d}{Y_{n+1}, \dots, Y_d} \right).$$

An explicit recursive formula for the SZ stuffle product $*_{\mathrm{SZ}}$ on the generating series of words $\rho_{\mathcal{B}}(\mathcal{W})$ is given in Proposition A.79.

2.3 Bi-brackets

We will consider the bi-brackets introduced by H. Bachmann ([Ba19]). They form a spanning set of the space $\mathcal{Z}_q$ and endow the algebra with weight and depth filtrations. There is only one infinite bi-alphabet, which describes the algebraic structure of the bi-brackets. The advantage of this model is that bi-brackets are closely related to quasi-modular forms and multiple Eisenstein series. In particular, one obtains that $\mathcal{Z}_q$ contains the algebra of quasi-modular forms.

Definition 2.27. For integers $k_1, \ldots, k_d \geq 1$ and $m_1, \ldots, m_d \geq 0$, the associated bi-bracket is

$$g\binom{k_1, \ldots, k_d}{m_1, \ldots, m_d} = \frac{1}{(k_1-1)! \ldots (k_d-1)!} \sum_{\substack{u_1 > \cdots > u_d > 0 \\ v_1, \ldots, v_d > 0}} u_1^{m_1} \ldots u_d^{m_d} v_1^{k_1-1} \ldots v_d^{k_d-1} q^{u_1 v_1 + \cdots + u_d v_d}$$
$$= \sum_{n_1 > \cdots > n_d > 0} n_1^{m_1} \ldots n_d^{m_d} \frac{P_{k_1}(q^{n_1})}{(1-q^{n_1})^{k_1}} \cdots \frac{P_{k_d}(q^{n_d})}{(1-q^{n_d})^{k_d}},$$

where the Eulerian polynomials $P_k(t) \in \mathbb{Q}[t],\ k \geq 1$, are defined by the equality

$$\frac{P_k(t)}{(1-t)^k} = \sum_{r \geq 1} \frac{r^{k-1}}{(k-1)!} t^r.$$

For a bi-index $\binom{k_1,\ldots,k_d}{m_1,\ldots,m_d} \in \mathbb{Z}_{\geq 0}^{2d}$, the weight and depth are defined by

$$\operatorname{wt}\binom{k_1, \ldots, k_d}{m_1, \ldots, m_d} = k_1 + \cdots + k_d + m_1 + \cdots + m_d,$$
$$\operatorname{dep}\binom{k_1, \ldots, k_d}{m_1, \ldots, m_d} = d.$$

We will also refer to this as the weight and depth of the bi-bracket $g\binom{k_1,\ldots,k_d}{m_1,\ldots,m_d}$. Moreover, denote

$$g(k_1, \ldots, k_d) = g\binom{k_1, \ldots, k_d}{0, \ldots, 0}$$

and we will refer to these q-series just as brackets.

Theorem 2.28. *([BK20, Theorem 2.3]) The following equalities hold*

$$\mathcal{Z}_q = \operatorname{span}_{\mathbb{Q}}\left\{ g\binom{k_1, \ldots, k_d}{m_1, \ldots, m_d} \;\middle|\; d \geq 0,\ k_1, \ldots, k_d \geq 1,\ m_1, \ldots, m_d \geq 0 \right\},$$
$$\mathcal{Z}_q^{\circ} = \operatorname{span}_{\mathbb{Q}}\{ g(k_1, \ldots, k_d) \mid d \geq 0,\ k_1, \ldots, k_d \geq 1 \}.$$

□

Here we set $g(\emptyset) = 1$.

By Theorem 2.28, the notions of weight and depth for bi-brackets define two compatible ascending filtrations on the space $\mathcal{Z}_q$

$$\operatorname{Fil}_W^{(w)}(\mathcal{Z}_q) = \operatorname{span}_{\mathbb{Q}}\left\{ g\binom{k_1, \ldots, k_d}{m_1, \ldots, m_d} \;\middle|\; \operatorname{wt}\binom{k_1, \ldots, k_d}{m_1, \ldots, m_d} \leq w \right\}, \tag{2.28.1}$$
$$\operatorname{Fil}_D^{(d)}(\mathcal{Z}_q) = \operatorname{span}_{\mathbb{Q}}\left\{ g\binom{k_1, \ldots, k_l}{m_1, \ldots, m_l} \;\middle|\; \operatorname{dep}\binom{k_1, \ldots, k_l}{m_1, \ldots, m_l} \leq d \right\}.$$

We will obtain in Corollary 2.39 that these filtrations coincide with the ones induced by the SZ multiple q-zeta values (2.10.1).

Brackets of depth 1 appear in the Fourier expansion of the Eisenstein series $G_k(\tau)$ for $k \geq 2$ even,

$$G_k(\tau) = -\frac{B_k}{2k!} + \frac{1}{(k-1)!}\sum_{n>0} \sigma_{k-1}(n)q^n = -\frac{B_k}{2k!} + g(k). \tag{2.28.2}$$

This definition of the Eisenstein series is non-standard, the usual definition is obtained by multiplying with the factor $(k-1)!$. To keep the notations and formulas short in the following, we will always use this normalization. There is also a formula for the Fourier expansion of multiple Eisenstein series in terms of brackets in arbitrary depth ([Ba20, Theorem 1.4]).

Since the Eisenstein series of weights 2, 4, and 6 generate the algebra of quasi-modular forms, Theorem 2.28 and (2.28.2) imply the following.

Proposition 2.29. *The algebra $\mathcal{Z}_q$ contains the algebra $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$ of quasi-modular forms with rational coefficients.*

Moreover, the bi-brackets are (modified) q-analogs of multiple zeta values.

Proposition 2.30. *(i) ([BI22, Section 4.1]) For all $k_1, \dots, k_d \geq 1$, $m_1, \dots, m_d \geq 0$, one has (possibly after some regularization process)*

$$\lim_{q \to 1} (1-q)^{k_1+\dots+k_d} g\binom{k_1, \dots, k_d}{m_1, \dots, m_d} \in \mathcal{Z}.$$

Here $\mathcal{Z}$ denotes the algebra of multiple zeta values (Definition B.1).

(ii) ([Zu15, Proposition 1]) For $k_1 \geq m_1 + 2$ and $k_i \geq m_i + 1$, $i = 2, \dots, d$, one obtains

$$\lim_{q \to 1} (1-q)^{k_1+\dots+k_d} g\binom{k_1, \dots, k_d}{m_1, \dots, m_d} = \zeta(k_1 - m_1, \dots, k_d - m_d).$$

□

The usual power series multiplication in $\mathcal{Z}_q$ can be expressed in terms of the bi-brackets, we refer to this expression as the product of bi-brackets. It can be described in terms of the following quasi-shuffle algebra (cf Subsection A.3).

Definition 2.31. Consider the bi-alphabet $\mathcal{Y}^{\mathrm{bi}} = \{y_{k,m} \mid k \geq 1,\ m \geq 0\}$ and let $\mathbb{Q}\langle \mathcal{Y}^{\mathrm{bi}} \rangle$ be the free non-commutative algebra generated by $\mathcal{Y}^{\mathrm{bi}}$. Moreover, denote the empty word by $\mathbf{1}$. Define the numbers

$$\lambda_j^{k_1,k_2} = -\left((-1)^{k_1}\binom{k_1+k_2-1-j}{k_2-j} + (-1)^{k_2}\binom{k_1+k_2-1-j}{k_1-j}\right)\frac{B_{k_1+k_2-j}}{(k_1+k_2-j)!} \in \mathbb{Q} \tag{2.31.1}$$

and set

$$y_{k_1,m_1} \diamond_{\mathrm{bb}} y_{k_2,m_2} = y_{k_1+k_2,m_1+m_2} + \sum_{j=1}^{k_1+k_2-1} \lambda_j^{k_1,k_2} y_{j,m_1+m_2}.$$

The product $\diamond_{\mathrm{bb}}$ is commutative and by [Ba19, Theorem 3.6] also associative. We denote the corresponding quasi-shuffle product on $\mathbb{Q}\langle \mathcal{Y}^{\mathrm{bi}} \rangle$ by $*_{\mathrm{bb}}$.

Define the weight and the depth of a word in $\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle$ as

$$\begin{aligned}\mathrm{wt}(y_{k_1,m_1}\dots y_{k_d,m_d}) &= k_1+\dots+k_d+m_1+\dots+m_d,\\ \mathrm{dep}(y_{k_1,m_1}\dots y_{k_d,m_d}) &= d.\end{aligned}$$

The algebra $(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *_{\mathrm{bb}})$ is bi-filtered with respect to weight and depth.

Theorem 2.32. *([Ba19, Theorem 3.6]) The map*

$$\begin{aligned}g:(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *_{\mathrm{bb}}) &\to (\mathcal{Z}_q,\cdot),\\ y_{k_1,m_1}\dots y_{k_d,m_d} &\mapsto g\binom{k_1,\dots,k_d}{m_1,\dots,m_d}\end{aligned}$$

is a surjective algebra morphism compatible with the weight and depth filtrations. □

If $k_1\geq 1,\ k_2,\dots,k_d\geq 1$ and $m_1=\dots=m_d=0$, then applying the limit $q\to 1$ (and multiplying with a suitable power of $(1-q)$) in Theorem 2.32 yields the stuffle product formula for multiple zeta values (Proposition B.20).

To describe another kind of relations satisfied by the bi-brackets, it is convenient to consider generating series. For each $d\geq 1$, define the generating series of the bi-brackets of depth d by

$$\mathfrak{g}_d\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} = \sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}} g\binom{k_1,\dots,k_d}{m_1,\dots,m_d} X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\dots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!} \tag{2.32.1}$$

and further set $\mathfrak{g}_0=1$.

Lemma 2.33. *([Ba19, Theorem 2.3]) For each $d\geq 1$, one has*

$$\begin{aligned}\mathfrak{g}_d\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} &= \sum_{\substack{u_1>\dots>u_d>0\\ v_1,\dots,v_d>0}}\prod_{i=1}^{d}\exp(v_iX_i)\exp(u_iY_i)q^{u_iv_i}\\ &= \sum_{u_1>\dots>u_d>0} L_{u_1}\binom{X_1}{Y_1}\dots L_{u_d}\binom{X_d}{Y_d},\end{aligned}$$

where

$$L_u\binom{X}{Y} = \frac{\exp(X+uY)q^u}{1-\exp(X)q^u},\qquad u\geq 1.$$ □

Interpreting the bi-brackets as generating series of polynomial functions on partitions (cf Proposition 2.8) gives linear relations among them.

Theorem 2.34. *([Ba19, Theorem 2.3]) For each $d\geq 1$, the generating series $\mathfrak{g}_d$ is swap invariant, i.e., the following holds*

$$\mathfrak{g}_d\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} = \mathfrak{g}_d\binom{Y_1+\dots+Y_d,\dots,Y_1+Y_2,Y_1}{X_d,X_{d-1}-X_d,\dots,X_1-X_2}.$$ □

Similar to Conjecture 2.22, the following is expected for the bi-brackets.

Conjecture 2.35. *([BK20], [Ba19]) All relations in $\mathcal{Z}_q$ are a consequence of the product formula (Theorem 2.32) and the swap invariance (Theorem 2.34) of the bi-brackets.*

We also want to describe the product of the bi-brackets $*_{\mathrm{bb}}$ in terms of generating series (cf Subsection A.4). Consider the generating series of words in $\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle$ given by $\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_0=\mathbf{1}$ and

$$\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_d\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}=\sum_{\substack{k_1,\dots,k_d\geq 1\\m_1,\dots,m_d\geq 0}}y_{k_1,m_1}\dots y_{k_d,m_d}X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\dots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!},\quad d\geq 1.$$

For simplicity, we often drop the depth index and just write $\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}$.

Extend the product $*_{\mathrm{bb}}$ and the bi-brackets map $g:\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle\to\mathcal{Z}_q$ from Theorem 2.32 by $\mathbb{Q}[[X_1,Y_1,X_2,Y_2,\dots]]$-linearity to $\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle[[X_1,Y_1,X_2,Y_2,\dots]]$. Then, one obtains by definition that for all $d\geq 1$

$$g\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_d\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}\right)=\mathfrak{g}_d\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}.$$

The map $g:(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle,*_{\mathrm{bb}})\to(\mathcal{Z}_q,\cdot)$ is an algebra morphism (Theorem 2.32), this implies the following.

Proposition 2.36. *For all* $0<n<d$, *one has*

$$\mathfrak{g}_n\begin{pmatrix}X_1,\dots,X_n\\Y_1,\dots,Y_n\end{pmatrix}\mathfrak{g}_{d-n}\begin{pmatrix}X_{n+1},\dots,X_d\\Y_{n+1},\dots,Y_d\end{pmatrix}$$
$$=g\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n\begin{pmatrix}X_1,\dots,X_n\\Y_1,\dots,Y_n\end{pmatrix}*_{\mathrm{bb}}\ \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_{d-n}\begin{pmatrix}X_{n+1},\dots,X_d\\Y_{n+1},\dots,Y_d\end{pmatrix}\right).$$

In particular, we want to describe the product $*_{\mathrm{bb}}$ explicitly on the generating series of words $\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})$. From [Ba19, Lemma 3.2] one deduces the following.

Proposition 2.37. *Set*

$$\mathfrak{b}(X)=\frac{1}{2}\left(\frac{1}{X}-\frac{1}{e^X-1}-\frac{1}{2}\right)=-\sum_{k\geq 2}\frac{B_k}{2k!}X^{k-1},\tag{2.37.1}$$

where B_k *denotes the* k*-th Bernoulli number. Then for all* $0<n<d$ *one has* $\mathbf{1}*_{\mathrm{bb}}\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n=\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n*_{\mathrm{bb}}\mathbf{1}=\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n$ *and*

$$\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_1,\dots,X_n\\Y_1,\dots,Y_n\end{pmatrix}*_{\mathrm{bb}}\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+1},\dots,X_d\\Y_{n+1},\dots,Y_d\end{pmatrix}$$
$$=\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_1\\Y_1\end{pmatrix}\cdot\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_2,\dots,X_n\\Y_2,\dots,Y_n\end{pmatrix}*_{\mathrm{bb}}\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+1},\dots,X_d\\Y_{n+1},\dots,Y_d\end{pmatrix}\right)$$
$$+\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+1}\\Y_{n+1}\end{pmatrix}\cdot\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_1,\dots,X_n\\Y_1,\dots,Y_n\end{pmatrix}*_{\mathrm{bb}}\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+2},\dots,X_d\\Y_{n+2},\dots,Y_d\end{pmatrix}\right)$$
$$+\Bigg(\left(\frac{1}{X_1-X_{n+1}}-2\mathfrak{b}(X_1-X_{n+1})\right)\cdot\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_1\\Y_1+Y_{n+1}\end{pmatrix}-\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+1}\\Y_1+Y_{n+1}\end{pmatrix}\right)$$
$$-\frac{1}{2}\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_1\\Y_1+Y_{n+1}\end{pmatrix}-\frac{1}{2}\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+1}\\Y_1+Y_{n+1}\end{pmatrix}\Bigg)$$
$$\cdot\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_2,\dots,X_n\\Y_2,\dots,Y_n\end{pmatrix}*_{\mathrm{bb}}\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+2},\dots,X_d\\Y_{n+2},\dots,Y_d\end{pmatrix}\right).$$

□

Here $\cdot$ denotes the usual concatenation product, by Proposition A.66 it is given for all $0 \leq n \leq d$ by

$$\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} \cdot \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d} = \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}.$$

In analogy to Theorem 2.21, combining the swap invariance of the bi-brackets (Theorem 2.34) and the product $*_{\mathrm{bb}}$ yields a second expression for the product of the generating series $\mathfrak{g}_d$. E.g., one has

$$\begin{aligned}
\mathfrak{g}_1\binom{X_1}{Y_1}\mathfrak{g}_1\binom{X_2}{Y_2} &= \mathfrak{g}_2\binom{X_1+X_2, X_1}{Y_2, Y_1-Y_2} + \mathfrak{g}_2\binom{X_1+X_2, X_2}{Y_1, Y_2-Y_1} \\
&\quad + \left(\frac{1}{Y_1-Y_2} - 2\mathfrak{b}(Y_1-Y_2)\right)\left(\mathfrak{g}_1\binom{X_1+X_2}{Y_1} - \mathfrak{g}_1\binom{X_1+X_2}{Y_2}\right) \\
&\quad - \frac{1}{2}\mathfrak{g}_1\binom{X_1+X_2}{Y_1} - \frac{1}{2}\mathfrak{g}_1\binom{X_1+X_2}{Y_2}.
\end{aligned}$$

This formula is a q-analog of the shuffle product for double zeta values. Explicitly, for $Y_1 = Y_2 = 0$ taking the limit $q \to 1$ (after multiplying with suitable powers of $(1-q)$) gives the shuffle product written in terms of generating series (Proposition B.42).

2.4 Comparison of SZ multiple q-zeta values and bi-brackets

In the previous two subsections, two different spanning sets of $\mathcal{Z}_q$ were presented, the SZ multiple q-zeta values (2.2) and the bi-brackets (2.3). In particular, there is a translation map from one spanning set into the other. We will give explicit formulas relating the generating series of SZ multiple q-zeta values $\mathfrak{sz}$ and bi-brackets $\mathfrak{g}$. The formulas will show that the weight and depth filtrations induced by these two spanning sets agree. Similar to [Br21, Theorem 2.41], we obtain the following.

Proposition 2.38. *For each $d \geq 1$, we have*

$$\begin{aligned}\mathfrak{g}_d\begin{pmatrix}X_1,\dots,X_d\\ Y_1,\dots,Y_d\end{pmatrix} &= \prod_{i=1}^{d}\exp(X_i)\exp(Y_1+\dots+Y_i)\\ &\quad\cdot\mathfrak{sz}_d\begin{pmatrix}\exp(X_1)-1,\exp(X_2)-1,\dots,\exp(X_d)-1\\ \exp(Y_1)-1,\exp(Y_1+Y_2)-1,\dots,\exp(Y_1+\dots+Y_d)-1\end{pmatrix},\\ \mathfrak{sz}_d\begin{pmatrix}X_1,\dots,X_d\\ Y_1,\dots,Y_d\end{pmatrix} &= \prod_{i=1}^{d}\frac{1}{(X_i+1)(Y_i+1)}\\ &\quad\cdot\mathfrak{g}_d\begin{pmatrix}\ln(X_1+1),\ln(X_2+1),\dots,\ln(X_d+1)\\ \ln(Y_1+1),\ln(Y_2+1)-\ln(Y_1+1),\dots,\ln(Y_d+1)-\ln(Y_{d-1}+1)\end{pmatrix}.\end{aligned}$$

Proof. Lemma 2.24 and 2.33 imply that we need to substitute

$$(1+X_i)^{v_i-1}(1+Y_i)^{u_i-u_{i+1}-1},\qquad \exp(X_i)^{v_i}\exp(Y_i)^{u_i}.$$

by each other for $i=1,\dots,d$. To get rid of the shift in the exponents by 1, there are additional factors in both equalities. Then the first equality follows from the substitution

$$X_i\mapsto\exp(X_i)-1,\quad Y_i\mapsto\exp(Y_1+\dots+Y_i)-1$$

and the second equality follows from the reversed substitution

$$X_i\to\ln(X_i+1),\ Y_i\mapsto\ln(Y_i+1)-\ln(Y_{i-1}+1)$$

(with $Y_0:=0$). □

One verifies directly that the formulas in Proposition 2.38 are compatible with the product formulas for SZ multiple q-zeta values (Proposition 2.26) and the bi-brackets (Proposition 2.36) and that they translate between τ-invariance of the SZ multiple q-zeta values (Proposition 2.25) and swap invariance of the bi-brackets (Theorem 2.34).

Corollary 2.39. *The notions of weight and depth for SZ multiple q-zeta values* (2.10.1) *and bi-brackets* (2.28.1) *induce the same filtrations on the algebra $\mathcal{Z}_q$, i.e., we obtain*

$$\begin{aligned}\mathrm{Fil}_W^{(w)}(\mathcal{Z}_q) &= \mathrm{span}_{\mathbb{Q}}\{\zeta_q^{\mathrm{SZ}}(k_1,\{0\}^{m_1}\dots,k_d,\{0\}^{m_d})\mid k_1+\dots+k_d+m_1+\dots+m_d\leq w\}\\ &= \mathrm{span}_{\mathbb{Q}}\left\{g\begin{pmatrix}k_1,\dots,k_d\\ m_1,\dots,m_d\end{pmatrix}\,\middle|\, k_1+\dots+k_d+m_1+\dots+m_d\leq w\right\},\end{aligned}$$

$$\begin{aligned}\mathrm{Fil}_D^{(d)}(\mathcal{Z}_q) &= \mathrm{span}_{\mathbb{Q}}\{\zeta_q^{\mathrm{SZ}}(k_1,\{0\}^{m_1}\dots,k_l,\{0\}^{m_l})\mid l\leq d\}\\ &= \mathrm{span}_{\mathbb{Q}}\left\{g\begin{pmatrix}k_1,\dots,k_l\\ m_1,\dots,m_l\end{pmatrix}\,\middle|\, l\leq d\right\}.\end{aligned}$$

Proof. Coefficient comparison in Proposition 2.38 shows that any bi-bracket of weight w is a $\mathbb{Q}$-linear combination of SZ multiple q-zeta values of weight $\leq w$ and vice versa. The translation formulas in Proposition 2.38 are homogeneous for the depth, so the depth filtrations induced by the SZ multiple q-zeta values and the bi-brackets have to be equal. □

2.5 Combinatorial bi-multiple Eisenstein series

The quasi-shuffle algebra $(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *_{\mathrm{bb}})$ for the bi-brackets (Theorem 2.32) is a weight-filtered algebra. In analogy to the case of multiple zeta values, we are interested in a weight-graded spanning set of $\mathcal{Z}_q$. Thus it seems natural to consider the associated weight-graded algebra to $(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *_{\mathrm{bb}})$ (in the sense of Definition A.48).

Definition 2.40. Define the q-stuffle product $*$ on $\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle$ to be the quasi-shuffle product corresponding to

$$y_{k_1,m_1} \diamond y_{k_2,m_2} = y_{k_1+k_2,m_1+m_2}.$$

Then $(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *)$ is a weight-graded algebra, it is exactly the associated weight-graded algebra to $(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *_{\mathrm{bb}})$.

M. Hoffman obtained isomorphisms between all quasi-shuffle algebras defined over the same alphabet in [Hof00] (cf Theorem A.57), in particular, there is an algebra isomorphism

$$\exp_{*_{\mathrm{bb}}} \circ \log_* : (\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *) \to (\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *_{\mathrm{bb}}).$$

Thus, one gets a surjective algebra morphism

$$\begin{aligned}(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *) &\to (\mathcal{Z}_q, \cdot),\\ w &\mapsto g\big(\exp_{*_{\mathrm{bb}}} \circ \log_*(w)\big),\end{aligned}$$

where $g(w)$ denotes the image of $w \in \mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle$ under the morphism in Theorem 2.32. Unfortunately, these images $g\big(\exp_{*_{\mathrm{bb}}} \circ \log_*(w)\big)$ satisfy relations coming from some involution, which is not weight-graded. Thus, we will provide another construction for a spanning set of $\mathcal{Z}_q$, which satisfies the q-stuffle product formula and still the swap invariance. The elements of this spanning set are called combinatorial bi-multiple Eisenstein series, they were first introduced in [BB22]. The key ingredients for the construction are the bi-brackets (Subsection 2.3) and a rational solution of the extended double shuffle equations (Definition B.24, Theorem B.25). In the following we will briefly recall the construction as given in [BB22]. This will be done on the level of generating series, thus we will use the language of bimoulds introduced in Appendix C.

Definition 2.41. By Theorem B.25 and (B.25.1) there exists a solution to the extended double shuffle equations $b \in \mathsf{DM}_{-\frac{1}{24}}(\mathbb{Q})$ satisfying $(b \mid x_0^k x_1) = 0$ for $k \geq 1$ even. Decompose the element $b_* \in \mathbb{Q}\langle\langle\mathcal{Y}\rangle\rangle$ (see Definition B.24) into its homogeneous depth components,

$$b_* = \sum_{d \geq 0} b_*^{(d)}, \qquad b_*^{(d)} \in \mathbb{Q}\langle\langle\mathcal{Y}\rangle\rangle^{(d)}.$$

Apply the $\mathbb{Q}$-linear map

$$\begin{aligned}\mathbb{Q}\langle\langle\mathcal{Y}\rangle\rangle &\to \mathbb{Q}[[X_1, X_2, \ldots]],\\ y_{k_1} \ldots y_{k_d} &\mapsto X_1^{k_1-1} \ldots X_d^{k_d-1}\end{aligned}$$

to the elements $b_*^{(d)}$ to obtain power series $\mathfrak{b}_d(X_1, \ldots, X_d) \in \mathbb{Q}[[X_1, \ldots, X_d]]$ for all $d \geq 1$. Moreover set $\mathfrak{b}_0 = 1$, then $\mathfrak{b} = (\mathfrak{b}_d)_{d \geq 0}$ is a mould in $\mathrm{GARI}^{\mathrm{pow},\mathbb{Q}}$.

Due to the choice of b, we have $(b \mid x_0 x_1) = -\frac{1}{24} = -\frac{B_2}{2 \cdot 2!}$ and $(b \mid x_0^k x_1) = 0$ for $k \geq 1$ even, so $\mathfrak{b}_1$ coincides with the generating series given in (2.37.1). But in higher depths, the element $b \in \mathsf{DM}_{-\frac{1}{24}}(\mathbb{Q})$ is not unique. In the following, we will fix the mould $\mathfrak{b}$, so the whole construction of the combinatorial bi-multiple Eisenstein series will depend on this choice.

Definition 2.42. To the mould $\mathfrak{b}$ associate a bimould also denoted as $\mathfrak{b}$ by

$$\mathfrak{b}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{0\leq i\leq j\leq d} \gamma_i \mathfrak{b}_{j-i}(Y_1+\dots+Y_{j-i},\dots,Y_1+Y_2,Y_1)\mathfrak{b}_{d-j}(X_{j+1},\dots,X_d),$$

where the coefficients γ_i are defined by

$$\sum_{i\geq 0}\gamma_i T^i = \exp\left(\sum_{n\geq 2}\frac{(-1)^{n+1}}{n}\frac{B_n}{2n!}T^n\right).$$

Moreover, define the bimould $\widetilde{\mathfrak{b}} = (\widetilde{\mathfrak{b}}_d)_{d\geq 0}$ by $\widetilde{\mathfrak{b}}_0 = 1$ and

$$\widetilde{\mathfrak{b}}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{i=0}^{d}\frac{(-1)^i}{2^i i!}\mathfrak{b}_{d-i}\begin{pmatrix} X_{i+1},\dots,X_d \\ -Y_1,\dots,-Y_{d-i} \end{pmatrix}, \qquad d\geq 1.$$

Definition 2.43. For each $u\geq 1$, let $\mathfrak{L}^{(u)} = (\mathfrak{L}_d^{(u)})_{d\geq 0}$ be the bimould given by $\mathfrak{L}_0^{(u)} = 1$ and

$$\mathfrak{L}_d^{(u)}\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{j=1}^{d}\mathfrak{b}_{j-1}\begin{pmatrix} X_1-X_j,\dots,X_{j-1}-X_j \\ Y_1,\dots,Y_{j-1} \end{pmatrix} L_u\begin{pmatrix} X_j \\ Y_1+\dots+Y_d \end{pmatrix} \cdot \widetilde{\mathfrak{b}}_{d-j}\begin{pmatrix} X_d-X_j,\dots,X_{j+1}-X_j \\ Y_d,\dots,Y_{j+1} \end{pmatrix},$$

where the power series $L_u\binom{X}{Y}$ is defined as in Lemma 2.33 by

$$L_u\begin{pmatrix} X \\ Y \end{pmatrix} = \frac{\exp(X+uY)q^u}{1-\exp(X)q^u}, \qquad u\geq 1.$$

In particular, the depth 1 component of the bimould $\mathfrak{L}^{(u)}$ is equal to the power series L_u.

Definition 2.44. Define the bimould $\mathfrak{g}^* = (\mathfrak{g}^*_d)_{d\geq 0}$ by $\mathfrak{g}^*_0 = 1$ and

$$\mathfrak{g}^*_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{1\leq j\leq d \\ 0=d_0<d_1<\dots<d_{j-1}<d_j=d \\ u_1>\dots>u_j>0}} \prod_{i=1}^{j}\mathfrak{L}^{(u_i)}_{d_i-d_{i-1}}\begin{pmatrix} X_{d_{i-1}+1},\dots,X_{d_i} \\ Y_{d_{i-1}+1},\dots,Y_{d_i} \end{pmatrix}.$$

Definition 2.45. Let $\mathfrak{G} = (\mathfrak{G}_d)_{d\geq 0}$ be the mould product of $\mathfrak{g}^*$ and $\mathfrak{b}$, i.e., one has $\mathfrak{G}_0 = 1$ and

$$\mathfrak{G} = \mathrm{mu}(\mathfrak{g}^*, \mathfrak{b}).$$

The main result of [BB22] was the following.

Theorem 2.46. *[BB22, Theorem 6.5.] The bimould $\mathfrak{G}$ is symmetril and swap invariant.* □

Definition 2.47. For $k_1,\dots,k_d\geq 1$, $m_1,\dots,m_d\geq 0$ define the combinatorial bi-multiple Eisenstein series $G\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$ to be the (normalized) coefficients of the bimould $\mathfrak{G}$,

$$\mathfrak{G}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1 \\ m_1,\dots,m_d\geq 0}} G\begin{pmatrix} k_1,\dots,k_d \\ m_1,\dots,m_d \end{pmatrix} X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\dots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}.$$

As for the bi-brackets (Definition 2.27), we refer to the number $k_1+\cdots+k_d+m_1+\cdots+m_d$ as the weight of $G\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$ and to the number d as its depth. Moreover, the elements

$$G(k_1,\dots,k_d)=G\begin{pmatrix}k_1,\dots,k_d\\0,\dots,0\end{pmatrix},\qquad k_1,\dots,k_d\geq 1,$$

are called the combinatorial multiple Eisenstein series.

Example 2.48. 1) In depth 1, one obtains

$$\mathfrak{G}_1\begin{pmatrix}X_1\\Y_1\end{pmatrix}=\mathfrak{b}_1\begin{pmatrix}X_1\\Y_1\end{pmatrix}+\mathfrak{g}_1\begin{pmatrix}X_1\\Y_1\end{pmatrix}$$

and thus for $k\geq 1,\ m\geq 0$

$$G\begin{pmatrix}k\\m\end{pmatrix}=-\delta_{m,0}\frac{B_k}{2k!}-\delta_{k,1}\frac{B_{m+1}}{2(m+1)}+\frac{1}{(k-1)!}\sum_{u,v>0}u^m v^{k-1}q^{uv}.$$

In particular, the combinatorial Eisenstein series $G(k)$ for $k\geq 2$ even are exactly the classical Eisenstein series of weight k with rational coefficients (expressed in their Fourier expansion). Moreover, the combinatorial bi-Eisenstein series $G\binom{k}{m}$, $k+m\geq 2$ even, is essentially the m-th derivative of the classical Eisenstein series $G(k)$ and hence is also contained in the algebra $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$.

2) In depth 2, one has

$$\mathfrak{G}_2\begin{pmatrix}X_1,X_2\\Y_1,Y_2\end{pmatrix}=\mathfrak{g}_2\begin{pmatrix}X_1,X_2\\Y_1,Y_2\end{pmatrix}+\mathfrak{b}_1\begin{pmatrix}X_1-X_2\\Y_1\end{pmatrix}\mathfrak{g}_1\begin{pmatrix}X_2\\Y_1+Y_2\end{pmatrix}+\mathfrak{g}_1\begin{pmatrix}X_1\\Y_1+Y_2\end{pmatrix}\widetilde{\mathfrak{b}}_1\begin{pmatrix}X_2-X_1\\Y_2\end{pmatrix}$$
$$+\mathfrak{g}_1\begin{pmatrix}X_1\\Y_1\end{pmatrix}\mathfrak{b}_1\begin{pmatrix}X_2\\Y_2\end{pmatrix}+\mathfrak{b}_2\begin{pmatrix}X_1,X_2\\Y_1,Y_2\end{pmatrix}.$$

This formula also gives an explicit but rather complicated expression of the combinatorial bi-multiple Eisenstein series in terms of the rational coefficients of $\mathfrak{b}$ and the bi-brackets.

Proposition 2.49. *([BB22, Proposition 6.15.]) The combinatorial bi-multiple Eisenstein series form a spanning set of $\mathcal{Z}_q$.* □

By Proposition 2.49 the notions of weight and depth of the combinatorial bi-multiple Eisenstein series endow the algebra $\mathcal{Z}_q$ with two filtrations. By construction, these filtrations agree with the ones of the bi-brackets given in (2.28.1) and hence also with the ones in Corollary 2.39. Moreover, Theorem 2.46, the definition of the symmetrility (Definition C.13), and Proposition 2.49 imply the following.

Theorem 2.50. *There is a surjective algebra morphism*

$$G:(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle,*)\to(\mathcal{Z}_q,\cdot),$$
$$y_{k_1,m_1}\cdots y_{k_d,m_d}\mapsto G\begin{pmatrix}k_1,\dots,k_d\\m_1,\dots,m_d\end{pmatrix}.$$

As a reformulation of Conjecture 2.35, the following is expected for the combinatorial bi-multiple Eisenstein series.

Conjecture 2.51. *([BB22, Remark 6.11.]) All relations in $\mathcal{Z}_q$ are a consequence of the q-stuffle product formula (Theorem 2.50) and the swap invariance (Theorem 2.46) of the combinatorial bi-multiple Eisenstein series.*

Proposition 2.52. *If Conjecture 2.51 holds, then the algebra $\mathcal{Z}_q$ is graded by weight*

$$\mathcal{Z}_q = \bigoplus_{w \geq 0} \mathcal{Z}_q^{(w)}.$$

Here $\mathcal{Z}_q^{(w)}$ denotes the subspace of $\mathcal{Z}_q$ spanned by all combinatorial bi-multiple Eisenstein series of weight w.

Proof. This follows immediately from the observation that the q-stuffle product and also the swap operator are homogeneous for the weight. □

2.6 Balanced multiple q-zeta values

The combinatorial bi-multiple Eisenstein series can be viewed as a weight-graded analog of the bi-brackets, since they satisfy the associated weight-graded relations of the bi-brackets. Similarly, one could ask for a weight-graded version of the SZ multiple q-zeta values. To obtain these elements we will use the combinatorial bi-multiple Eisenstein series constructed in [BB22]. More precisely, we will obtain the weight-graded version of the SZ multiple q-zeta values by applying a linear variables substitution to the bimould $\mathfrak{G}$ of the generating series of the combinatorial bi-multiple Eisenstein series (Definition 2.45).

Definition 2.53. Let $\mathfrak{B} = (\mathfrak{B}_d)_{d\geq 0}$ be the bimould in GBARI given by $\mathfrak{B}_0 = 1$ and

$$\mathfrak{B}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \mathfrak{G}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1, Y_2-Y_1,\dots,Y_d-Y_{d-1} \end{pmatrix}, \qquad d\geq 1.$$

Remark 2.54. This definition has much similarities with Zudilin's definition of the multiple q-zeta brackets in terms of the bi-brackets ([Zu15, eq (8)]). Moreover, this definition should be seen as a weight-graded version of the comparison formula for the SZ multiple q-zeta values and the bi-brackets (Proposition 2.38).

Proposition 2.55. *The bimould $\mathfrak{B}$ is q-symmetril and τ-invariant.*

We will explain the resulting properties for the coefficients now and give the proof of the proposition later (Subsection 2.7).

Definition 2.56. For $k_1,\dots,k_d\geq 1,\ m_1,\dots,m_d\geq 0$ define the balanced multiple q-zeta values $\zeta_q(k_1,\{0\}^{m_1},\dots,k_d,\{0\}^{m_d})$ to be the coefficients of the bimould $\mathfrak{B}$,

$$\mathfrak{B}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1,\\ m_1,\dots,m_d\geq 0}} \zeta_q(k_1,\{0\}^{m_1},\dots,k_d,\{0\}^{m_d})X_1^{k_1-1}Y_1^{m_1}\dots X_d^{k_d-1}Y_d^{m_d}.$$

As for the SZ multiple q-zeta values (Definition 2.9), we call $s_1+\dots+s_l+\#\{i\mid s_i=0\}$ the weight and $l-\#\{i\mid s_i=0\}$ the depth of the balanced multiple q-zeta value $\zeta_q(s_1,\dots,s_l)$.

Proposition 2.57. *The balanced multiple q-zeta values form a spanning set of $\mathcal{Z}_q$.*

Proof. The combinatorial bi-multiple Eisenstein series form a spanning set of $\mathcal{Z}_q$ (Proposition 2.49). Since the translation between the combinatorial bi-multiple Eisenstein series and the balanced multiple q-zeta values given in Definition 2.53 is bijective, also the balanced multiple q-zeta values give a spanning set of $\mathcal{Z}_q$. □

In particular, by Proposition 2.57 the notions of weight and depth of the balanced multiple q-zeta values induce two filtrations on $\mathcal{Z}_q$. Since the transformation from the combinatorial bi-multiple Eisenstein series into the balanced multiple q-zeta values is given by a weight- and depth-homogeneous substitution (Definition 2.53), they coincide with the filtrations induced by the combinatorial bi-multiple Eisenstein series and thus also with the ones in Corollary 2.39.

Definition 2.58. Consider the alphabet $\mathcal{B}=\{b_0,b_1,b_2,\dots\}$ and define the balanced quasi-shuffle product $*_q$ on $\mathbb{Q}\langle\mathcal{B}\rangle$ to be the quasi-shuffle product corresponding to

$$b_i\diamond_q b_j = \begin{cases} b_{i+j} & \text{if } i,j\geq 1,\\ 0 & \text{else}\end{cases}.$$

We call the product $*_q$ balanced quasi-shuffle product, since it combines the well-known shuffle and stuffle product (Definition B.13, B.17) is a very simple way (cf (4.8.1)). By definition $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q)$ is the associated weight-graded algebra to quasi-shuffle algebra $(\mathbb{Q}\langle\mathcal{B}\rangle, *_{\mathrm{SZ}})$ introduced for the SZ multiple q-zeta values (Definition 2.11). Let $\mathbb{Q}\langle\mathcal{B}\rangle^0$ be the subalgebra of $\mathbb{Q}\langle\mathcal{B}\rangle$ spanned by all words, which do not start in b_0.

Theorem 2.59. *There is a τ-invariant surjective algebra morphism*

$$\begin{aligned}\zeta_q : (\mathbb{Q}\langle\mathcal{B}\rangle^0, *_q) &\to (\mathcal{Z}_q, \cdot),\\ b_{s_1}\dots b_{s_l} &\mapsto \zeta_q(s_1,\dots,s_l).\end{aligned}$$

Proof. The surjectivity follows from Proposition 2.57. By Proposition 2.55 and the definition of q-symmetrility (Definition 2.67), we obtain that the map is indeed an algebra morphism. Finally, Proposition 2.55 and the same calculations as in Theorem 2.25 show that the balanced multiple q-zeta values are τ-invariant. □

As a reformulation of Conjecture 2.22, we expect the following.

Conjecture 2.60. *All relations in $\mathcal{Z}_q$ are a consequence of the balanced quasi-shuffle product formula and the τ-invariance (Theorem 2.59) of the balanced multiple q-zeta values.*

If Conjecture 2.60 holds, then the algebra $\mathcal{Z}_q$ is graded by weight

$$\mathcal{Z}_q = \bigoplus_{w\geq 0} \mathcal{Z}_q^{(w)},$$

where $\mathcal{Z}_q^{(w)}$ is the subspace of $\mathcal{Z}_q$ spanned by all balanced multiple q-zeta values of weight w. This conjectural grading coincides with the one of the combinatorial bi-multiple Eisenstein series (Proposition 2.52).

Example 2.61. 1) By Example 2.68 and 2.72 the bimould $\mathfrak{B}$ satisfies the following relations in depth ≤ 2

$$\begin{aligned}\mathfrak{B}_1\binom{X_1}{Y_1}\cdot\mathfrak{B}_1\binom{X_2}{Y_2} &= \mathfrak{B}_2\binom{X_2, X_1}{Y_2, Y_1+Y_2} + \mathfrak{B}_2\binom{X_1, X_2}{Y_1, Y_1+Y_2} + \frac{\mathfrak{B}_1\binom{X_1}{Y_1+Y_2} - \mathfrak{B}_1\binom{X_2}{Y_1+Y_2}}{X_1-X_2}\\ &= \mathfrak{B}_2\binom{X_1+X_2, X_2}{Y_1, Y_2} + \mathfrak{B}_2\binom{X_1+X_2, X_1}{Y_2, Y_1} + \frac{\mathfrak{B}_1\binom{X_1+X_2}{Y_1} - \mathfrak{B}_1\binom{X_1+X_2}{Y_2}}{Y_1-Y_2}.\end{aligned}$$

Formalizing these equations, one gets a space closely related to the formal double Eisenstein space introduced and studied in [BKM21].

2) In depth 1 the balanced multiple q-zeta values coincide with the combinatorial bi-multiple Eisenstein series up to multiplying with some factorials. Thus we deduce from Example 2.48 1) that for all $k \geq 1,\ m \geq 0$

$$\zeta_q(k, \{0\}^m) = -\delta_{m,0}\frac{B_k}{2k!} - \delta_{k,1}\frac{B_{m+1}}{2(m+1)!} + \frac{1}{(k-1)!m!}\sum_{u,v>0} u^m v^{k-1} q^{uv}.$$

In particular, the element $\zeta_q(k)$, $k \geq 2$ even, equals the classical Eisenstein series of weight k and $\zeta_q(k, \{0\}^m)$, $k+m \geq 2$ even, is essentially equal to the m-th derivative of the Eisenstein series G_k.

If $k_1, \dots, k_d \geq 1$, then the balanced multiple q-zeta value $\zeta_q(k_1, \dots, k_d)$ equals the combinatorial multiple Eisenstein series $G(k_1, \dots, k_d)$.

3) Denote by $\beta(k_1, k_2)$ the coefficients of the depth 2 part of the mould $\mathfrak{b}$ (Definition 2.41), so $\mathfrak{b}(X_1, X_2) = \sum_{k_1,k_2 \geq 1} \beta(k_1, k_2) X_1^{k_1-1} X_2^{k_2-1}$. Then direct calculations show that

$$\zeta_q(2,3) = \beta(2,3) - \frac{1}{48} \sum_{u,v>0} v^2 q^{uv} + \frac{1}{2} \sum_{\substack{u_1>u_2>0 \\ v_1,v_2>0}} v_1 v_2^2 q^{u_1v_1+u_2v_2},$$

$$\zeta(2,0,3) = \frac{1}{2} \sum_{\substack{u_1>u_2>0 \\ v_1,v_2>0}} u_1 v_1 v_2^2 q^{u_1v_1+u_2v_2} - \frac{1}{2} \sum_{\substack{u_1>u_2>0 \\ v_1,v_2>0}} u_2 v_1 v_2^2 q^{u_1v_1+u_2v_2}.$$

An explicit construction for the numbers $\beta(k_1, k_2)$ is, for example, given in [GKZ06, Section 6], in this case, one has $\beta(2,3) = 0$. Other constructions for these rational numbers are given in [Bro17(2)] and [Ec02].

4) The quasi-modular forms are contained in the algebra $\mathcal{Z}_q$ (Proposition 2.29), in particular, the modular discriminant $\Delta = q \prod_{n\geq 1}(1-q^n)^{24}$ is a $\mathbb{Q}$-linear combination of balanced multiple q-zeta values. Precisely, we have

$$\frac{1}{43200}\Delta = 240\zeta_q(4,4,4) + 120\zeta_q(4,8) + 120\zeta_q(8,4) - 98\zeta_q(6,6) - 9\zeta_q(12).$$

As studied in [EMS16] and [Si15] for the SZ multiple zeta values (cf Theorem 2.18, 2.21), there is a second product defined on the non-commutative algebra $\mathbb{Q}\langle p, y\rangle$ describing the product of balanced multiple q-zeta values.

Definition 2.62. Let $ш_q$ be the product on the non-commutative free algebra $\mathbb{Q}\langle p, y\rangle$ recursively defined by $\mathbf{1} ш_q w = w ш_q \mathbf{1} = w$ and

$$(yu) ш_q v = u ш_q (yv) = y(u ш_q v),$$

$$(pu) ш_q (pv) = p(u ш_q pv) + p(pu ш_q v) + \begin{cases} p(u ш_q v), & \text{if } u = y\tilde{u} \text{ and } v = y\tilde{v}, \\ 0 & \text{else} \end{cases}$$

for all $u, v, w \in \mathbb{Q}\langle p, y\rangle$.

The involution $\tau : \mathbb{Q}\langle p, y\rangle \to \mathbb{Q}\langle p, y\rangle$ from Definition 2.20 relates the products $*_q$ and $ш_q$.

Proposition 2.63. *For all $u, v \in \mathbb{Q}\langle\mathcal{B}\rangle$, we have*

$$i(u *_q v) = \tau(\tau \circ i(u) ш_q \tau \circ i(v)),$$

where the embedding $i : \mathbb{Q}\langle\mathcal{B}\rangle \to \mathbb{Q}\langle p, y\rangle$ is defined in (2.20.1).

Proof. Let $u = b_{s_1} \dots b_{s_l}$ and $v = b_{r_1} \dots b_{r_k}$ be words in $\mathbb{Q}\langle\mathcal{B}\rangle$ and $s_l, r_k \geq 1$. Since $*_q$ is a quasi-shuffle product, it can be equally defined recursively from the right. Thus, we obtain

$$\begin{aligned} i(u *_q v) = {} & i(b_{s_1} \dots b_{s_{l-1}} *_q b_{r_1} \dots b_{r_k}) p^{s_l} y + i(b_{s_1} \dots b_{s_l} *_q b_{r_1} \dots b_{r_{k-1}}) p^{r_k} y \\ & + i(b_{s_2} \dots b_{s_l} *_q b_{r_2} \dots b_{r_k}) p^{s_l + r_k} y \end{aligned}$$

and on the other hand

$$
\begin{aligned}
&\tau(\tau\circ i(u)\sqcup\!\sqcup_q \tau\circ i(v)) = \tau(py^{s_l}\dots py^{s_1}\sqcup\!\sqcup_q py^{r_k}\dots py^{s_1})\\
&\quad = \tau\Big(py^{s_l}(py^{s_{l-1}}\dots py^{s_1}\sqcup\!\sqcup_q py^{r_k}\dots py^{r_1}) + py^{r_k}(py^{s_l}\dots py^{s_1}\sqcup\!\sqcup_q py^{r_{k-1}}\dots py^{r_1})\\
&\qquad + py^{s_l+r_k}(py^{s_{l-1}}\dots py^{s_1}\sqcup\!\sqcup_q py^{r_{k-1}}\dots py^{r_1})\Big)\\
&\quad = \tau\Big(\tau\circ i(b_{s_1}\dots b_{s_{l-1}})\sqcup\!\sqcup_q \tau\circ i(b_{r_1}\dots b_{r_k})\Big)p^{s_l}y\\
&\qquad + \tau\Big(\tau\circ i(b_{s_1}\dots b_{s_l})\sqcup\!\sqcup_q \tau\circ i(b_{r_1}\dots b_{r_{k-1}})\Big)p^{r_k}y\\
&\qquad + \tau\Big(\tau\circ i(b_{s_1}\dots b_{s_{l-1}})\sqcup\!\sqcup_q \tau\circ i(b_{r_1}\dots b_{r_{k-1}})\Big)p^{s_l+r_k}y
\end{aligned}
$$

Next, assume that $s_l = 0$ and $r_k \geq 0$. Then we obtain

$$
i(u *_q v) = i(b_{s_1}\dots b_{s_{l-1}} *_q b_{r_1}\dots b_{r_k})y + i(b_{s_1}\dots b_{s_l} *_q b_{r_1}\dots b_{r_{k-1}})p^{r_k}y
$$

and

$$
\begin{aligned}
&\tau(\tau\circ i(u)\sqcup\!\sqcup_q \tau\circ i(v)) = \tau(py^{s_l}\dots py^{s_1}\sqcup\!\sqcup_q py^{r_k}\dots py^{r_1})\\
&\quad = \tau\Big(p(py^{s_{l-1}}\dots py^{s_1}\sqcup\!\sqcup_q py^{r_k}\dots py^{r_1}) + py^{r_k}(py^{s_l}\dots py^{s_1}\sqcup\!\sqcup_q py^{r_{k-1}}\dots py^{r_1})\Big)\\
&\quad = \tau\Big(\tau\circ i(b_{s_1}\dots b_{s_{l-1}})\sqcup\!\sqcup_q \tau\circ i(b_{r_1}\dots b_{r_k})\Big)y\\
&\qquad + \tau\Big(\tau\circ i(b_{s_1}\dots b_{s_l})\sqcup\!\sqcup_q \tau\circ i(b_{r_1}\dots b_{r_{k-1}})\Big)p^{r_k}y
\end{aligned}
$$

In both cases, induction on the length of the words implies the claim. ☐

By Proposition 2.63, there is injective algebra morphism

$$
\begin{aligned}
\tau\circ i : (\mathbb{Q}\langle\mathcal{B}\rangle, *_q) &\hookrightarrow (\mathbb{Q}\langle p,y\rangle, \sqcup\!\sqcup_q),\\
b_{s_1}\dots b_{s_l} &\mapsto py^{s_l}\dots py^{s_1}.
\end{aligned}
\tag{2.63.1}
$$

In particular, the restriction of $\sqcup\!\sqcup_q$ to $\mathrm{im}(\tau\circ i) = \mathbb{Q}\mathbf{1} + p\mathbb{Q}\langle p,y\rangle$ can be seen as a quasi-shuffle product. Denote

$$
\mathbb{Q}\langle p,y\rangle^0 = \mathbb{Q}\mathbf{1} + p\mathbb{Q}\langle p,y\rangle y.
$$

Theorem 2.64. *There is a surjective algebra morphism*

$$
\begin{aligned}
(\mathbb{Q}\langle p,y\rangle^0, \sqcup\!\sqcup_q) &\to (\mathcal{Z}_q, \cdot),\\
p^{s_1}y\dots p^{s_l}y &\mapsto \zeta_q(s_1,\dots,s_l).
\end{aligned}
$$

Proof. First, observe that by definition $\zeta_q(i(u)) = \zeta_q(u)$ for all $u \in \mathbb{Q}\langle\mathcal{B}\rangle^0$. So for $s_1, r_1 \geq 1,\ s_2,\dots,s_l,r_2,\dots,r_k \geq 0$, we compute with Theorem 2.59 and Proposition 2.63

$$
\begin{aligned}
\zeta_q(py^{s_l}\dots py^{s_1})\zeta_q(py^{r_k}\dots py^{r_1}) &= \zeta_q(p^{s_1}y\dots p^{s_l}y)\zeta_q(p^{r_1}y\dots p^{r_k}y)\\
&= \zeta_q(b_{s_1}\dots b_{s_l})\zeta_q(b_{r_1}\dots b_{r_k})\\
&= \zeta_q(b_{s_1}\dots b_{s_l} *_q b_{r_1}\dots b_{r_k})\\
&= \zeta_q(\tau(\tau\circ i(b_{s_1}\dots b_{s_l})\sqcup\!\sqcup_q \tau\circ i(b_{r_1}\dots b_{r_k})))\\
&= \zeta_q(\tau\circ i(b_{s_1}\dots b_{s_l})\sqcup\!\sqcup_q \tau\circ i(b_{r_1}\dots b_{r_k}))\\
&= \zeta_q(py^{s_l}\dots py^{s_1}\sqcup\!\sqcup_q py^{r_k}\dots py^{r_1}).
\end{aligned}
$$

Surjectivity is a direct consequence of Proposition 2.57. ☐

2.7 Comparing the symmetries of $\mathfrak{G}$ and $\mathfrak{B}$

We will explain the symmetries of bimoulds, which occur particularly in the context of the balanced multiple q-zeta values. We are interested in a very explicit and detailed description of them. Then we will relate these symmetries to the ones of the bimould $\mathfrak{G}$ (Theorem 2.46) and this will give the proof of Proposition 2.55. An introductory overview of bimoulds is given in Appendix C. All bimoulds in the following will have coefficients in some fixed commutative $\mathbb{Q}$-algebra R with unit. Moreover, the components of all bimoulds considered in the following are power series or polynomials. In particular, we will drop the indices indicating the underlying $\mathbb{Q}$-algebra and the shape of the components.

Definition 2.65. For a bimould $A \in \mathrm{BIMU}$, define the bimould $\tau(A)$ by

$$\tau(A)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = A\begin{pmatrix} Y_d,\dots,Y_1 \\ X_d,\dots,X_1 \end{pmatrix}.$$

We call a bimould A τ-invariant if $\tau(A) = A$.

Let $A \in \mathrm{BIMU}$ be a bimould and write for all $d \geq 1$

$$A\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1 \\ m_1,\dots,m_d\geq 0}} a\begin{pmatrix} k_1,\dots,k_d \\ m_1,\dots,m_d \end{pmatrix} X_1^{k_1-1}\dots X_d^{k_d-1}Y_1^{m_1}\dots Y_d^{m_d}.$$

Then A is τ-invariant if and only if

$$a\begin{pmatrix} k_1,\dots,k_d \\ m_1,\dots,m_d \end{pmatrix} = a\begin{pmatrix} m_d+1,\dots,m_1+1 \\ k_d-1,\dots,k_1-1 \end{pmatrix} \tag{2.65.1}$$

for all $k_1,\dots,k_d \geq 1$ and $m_1,\dots,m_d \geq 0$.

We want to translate the shuffle product and the balanced quasi-shuffle product defined on $\mathbb{Q}\langle\mathcal{B}\rangle$ into the language of bimoulds by applying the general setup introduced in A.4. Recall that the depth of a word in $\mathbb{Q}\langle\mathcal{B}\rangle^0$ is defined by $\mathrm{dep}(b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d}) = d$ for all $k_1,\dots,k_d \geq 1,\ m_1,\dots,m_d \geq 0$. A $\mathbb{Q}$-linear map $\rho_{\mathcal{B}}$ satisfying the conditions in Definition A.64 is given by

$$\begin{aligned} \rho_{\mathcal{B}}: \mathbb{Q}\langle\mathcal{B}\rangle^0 &\to \mathbb{Q}[X_1,Y_1,X_2,Y_2,\dots], \\ b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d} &\mapsto X_1^{k_1-1}Y_1^{m_1}\dots X_d^{k_d-1}Y_d^{m_d} \quad (k_1,\dots,k_d\geq 1, m_1,\dots,m_d\geq 0). \end{aligned}$$

The generating series of words in $\mathbb{Q}\langle\mathcal{B}\rangle^0$ associated to $\rho_{\mathcal{B}}$ is given by $\rho_{\mathcal{B}}(\mathcal{W})_0 = \mathbf{1}$ and for $d \geq 1$ by

$$\rho_{\mathcal{B}}(\mathcal{W})_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1 \\ m_1,\dots,m_d\geq 0}} b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d}X_1^{k_1-1}Y_1^{m_1}\dots X_d^{k_d-1}Y_d^{m_d}. \tag{2.65.2}$$

Definition 2.66. Let $\sqcup\!\sqcup$ be the shuffle product on $\mathbb{Q}\langle\mathcal{B}\rangle^0$, i.e., the quasi-shuffle product with $b_i \diamond b_j = 0$ (Example A.53, 1)). A bimould $A \in \mathrm{GBARI}$ is called q-symmetral if there is an algebra morphism $\varphi_{\sqcup\!\sqcup}: (\mathbb{Q}\langle\mathcal{B}\rangle^0, \sqcup\!\sqcup) \to R$, such that for all $d \geq 1$

$$A_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1 \\ m_1,\dots,m_d\geq 0}} \varphi_{\sqcup\!\sqcup}(b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d})X_1^{k_1-1}Y_1^{m_1}\dots X_d^{k_d-1}Y_d^{m_d}.$$

In other words, A is q-symmetral if and only if it is $(\varphi_{\sqcup\!\sqcup}, \rho_{\mathcal{B}})$-symmetric in the sense of Definition A.71. We will refer to the map $\varphi_{\sqcup\!\sqcup}$ as the coefficient map of A.

The subset of all q-symmetral bimoulds is denoted by $\mathrm{GBARI}_{q\text{-as}}$.

According to (A.71.1) a bimould $A \in \mathrm{GBARI}$ is q-symmetral with coefficient map $\varphi_{ш}$ if and only if for all $0 < n < d$

$$A\begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} A\begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix} = \varphi_{ш}\left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} ш \, \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix}\right).$$

An explicit recursive formula for ш on the generating series of words $\rho_{\mathcal{B}}(\mathcal{W})$ is given in Proposition A.78 (i).

Definition 2.67. Consider the balanced quasi-shuffle product $*_q$ on $\mathbb{Q}\langle\mathcal{B}\rangle^0$, i.e., the quasi-shuffle product with $b_i \diamond_q b_j = \begin{cases} b_{i+j}, & i, j \geq 1 \\ 0 & \text{else} \end{cases}$ (Definition 2.58). A bimould $A \in \mathrm{GBARI}$ is called q-symmetril if there is an algebra morphism $\varphi_{*_q} : (\mathbb{Q}\langle\mathcal{B}\rangle^0, *_q) \to R$, such that for all $d \geq 1$

$$A_d\begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix} = \sum_{\substack{k_1, \dots, k_d \geq 1 \\ m_1, \dots, m_d \geq 0}} \varphi_{*_q}(b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}) X_1^{k_1 - 1} Y_1^{m_1} \dots X_d^{k_d - 1} Y_d^{m_d}.$$

So A is q-symmetril if and only if A is $(\varphi_{*_q}, \rho_{\mathcal{B}})$-symmetric. As before, we call the map φ_{*_q} also the coefficient map of A.

Denote the subset of all q-symmetril bimoulds by $\mathrm{GBARI}_{q\text{-is}}$.

A bimould $A \in \mathrm{GBARI}$ is q-symmetril with coefficient map φ_{*_q} if and only if for all $0 < n < d$

$$A\begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} A\begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix} = \varphi_{*_q}\left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} *_q \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix}\right).$$

An explicit recursive formula for the balanced quasi-shuffle product $*_q$ on the generating series of words $\rho_{\mathcal{B}}(\mathcal{W})$ is given in Proposition A.78 (ii).

Example 2.68. For a bimould $A \in \mathrm{GBARI}$, q-symmetrility in depth 2 and 3 means

$$\begin{aligned} A\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} \cdot A\begin{pmatrix} X_2 \\ Y_2 \end{pmatrix} &= A\begin{pmatrix} X_2, X_1 \\ Y_2, Y_1 + Y_2 \end{pmatrix} + A\begin{pmatrix} X_1, X_2 \\ Y_1, Y_1 + Y_2 \end{pmatrix} \\ &\quad + \frac{1}{X_1 - X_2}\left(A\begin{pmatrix} X_1 \\ Y_1 + Y_2 \end{pmatrix} - A\begin{pmatrix} X_2 \\ Y_1 + Y_2 \end{pmatrix}\right), \\ A\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} \cdot A\begin{pmatrix} X_2, X_3 \\ Y_2, Y_3 \end{pmatrix} &= A\begin{pmatrix} X_2, X_3, X_1 \\ Y_2, Y_3, Y_1 + Y_3 \end{pmatrix} + A\begin{pmatrix} X_2, X_1, X_3 \\ Y_2, Y_1 + Y_2, Y_1 + Y_3 \end{pmatrix} \\ &\quad + A\begin{pmatrix} X_1, X_2, X_3 \\ Y_1, Y_1 + Y_2, Y_1 + Y_3 \end{pmatrix} + \frac{1}{X_1 - X_3}\left(A\begin{pmatrix} X_2, X_1 \\ Y_2, Y_1 + Y_3 \end{pmatrix} - A\begin{pmatrix} X_2, X_3 \\ Y_2, Y_1 + Y_3 \end{pmatrix}\right) \\ &\quad + \frac{1}{X_1 - X_2}\left(A\begin{pmatrix} X_1, X_3 \\ Y_1 + Y_2, Y_1 + Y_3 \end{pmatrix} - A\begin{pmatrix} X_2, X_3 \\ Y_1 + Y_2, Y_1 + Y_3 \end{pmatrix}\right). \end{aligned}$$

Omit all terms of lower depths to obtain the formulas for q-symmetrality in depths ≤ 3.

Definition 2.69. Define the following subsets of GBARI,

$$\mathrm{GBARI}_{q\text{-as},\tau} = \{A \in \mathrm{GBARI} \mid A\ q\text{-symmetral and } \tau\text{-invariant}\},$$
$$\mathrm{GBARI}_{q\text{-is},\tau} = \{A \in \mathrm{GBARI} \mid A\ q\text{-symmetril and } \tau\text{-invariant}\}.$$

The bimoulds in these two subsets also satisfy a second product formula. For $\mathrm{GBARI}_{q\text{-is},\tau}$ we will give an explicit description, then consider these formulas modulo lower depths to obtain the corresponding formulas for $\mathrm{GBARI}_{q\text{-as},\tau}$.

Definition 2.70. Define the product $*_\tau$ recursively on the generating series of words $\rho_{\mathcal{B}}(\mathcal{W})$ for $0 < n < d$ by $\mathbf{1} *_\tau \rho_{\mathcal{B}}(\mathcal{W})_n = \rho_{\mathcal{B}}(\mathcal{W})_n *_\tau \mathbf{1} = \rho_{\mathcal{B}}(\mathcal{W})_n$ and

$$\begin{aligned}
&\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_\tau \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}\\
&= \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1+X_{n+1}}{Y_1}\cdot\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2,\dots,X_n}{Y_2,\dots,Y_n} *_\tau \rho_{\mathcal{B}}(\mathcal{W})_{d-n}\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}\right)\\
&\quad+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1+X_{n+1}}{Y_{n+1}}\cdot\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_\tau \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+2},\dots,X_d}{Y_{n+2},\dots,Y_d}\right)\\
&\quad+\frac{\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1+X_{n+1}}{Y_1}-\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1+X_{n+1}}{Y_{n+1}}}{Y_1-Y_{n+1}}\\
&\qquad\qquad\cdot\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2,\dots,X_n}{Y_2,\dots,Y_n} *_\tau \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+2},\dots,X_d}{Y_{n+2},\dots,Y_d}\right).
\end{aligned}$$

Proposition 2.71. *A bimould $A \in \mathrm{GBARI}_{q\text{-is},\tau}$ satisfies for all $0 < n < d$*

$$\begin{aligned}
&A\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} A\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}\\
&\qquad= \varphi_{*_q}\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_\tau \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}\right),
\end{aligned}$$

where $\varphi_{*_q} : (\mathbb{Q}\langle\mathcal{B}\rangle^0, *_q) \to R$ is the coefficient map of A (cf Definition 2.67).

If A equals the bimould $\mathfrak{B}$ of the generating series of the balanced multiple q-zeta values, then Proposition 2.71 is equivalent to the second product formula of the balanced multiple q-zeta values given in Theorem 2.64.

Proof. Let $A \in \mathrm{GBARI}_{q\text{-is},\tau}$ and write for $d \geq 1$

$$A\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} = \sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}} a\binom{k_1,\dots,k_d}{m_1,\dots,m_d} X_1^{k_1-1}\dots X_d^{k_d-1}Y_1^{m_1}\dots Y_d^{m_d}.$$

Then

$$\mathbb{Q}\langle\mathcal{B}\rangle^0 \to R, \quad b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d} \mapsto a\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$$

is an algebra morphism for the balanced quasi-shuffle product $*_q$ and the coefficients $a\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$ satisfy the τ-invariance given in (2.65.1). So instead of simply multiplying two coefficients with respect to the balanced quasi-shuffle product, apply the τ-invariance to both factors then multiply with respect to the balanced quasi-shuffle product, and finally apply again the τ-invariance to all terms. Since A is an element in $\mathrm{GBARI}_{q\text{-is},\tau}$, this gives the same result. On the level of bimoulds, this means for $0 < n < d$

$$A\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} A\begin{pmatrix} X_{n+1},\dots,X_d \\ Y_{n+1},\dots,Y_d \end{pmatrix}$$
$$= \varphi_{*_q}\left(\tau\left(\tau\big(\rho_{\mathcal{B}}(\mathcal{W})\big)\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} *_q \tau\big(\rho_{\mathcal{B}}(\mathcal{W})\big)\begin{pmatrix} X_{n+1},\dots,X_d \\ Y_{n+1},\dots,Y_d \end{pmatrix}\right)\right).$$

Evaluating τ and $*_q$ (cf Proposition A.78 (ii)), we immediately see that the right hand side is equal to $\varphi_{*_q}\left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} *_\tau \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1},\dots,X_d \\ Y_{n+1},\dots,Y_d \end{pmatrix}\right)$. $\square$

Example 2.72. Expanding out the product $*_\tau$ in depths 2 and 3, we obtain that any bimould $A \in \mathrm{GBARI}_{q\text{-is},\tau}$ satisfies

$$A\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} \cdot A\begin{pmatrix} X_2 \\ Y_2 \end{pmatrix} = A\begin{pmatrix} X_1+X_2, X_2 \\ Y_1, Y_2 \end{pmatrix} + A\begin{pmatrix} X_1+X_2, X_1 \\ Y_2, Y_1 \end{pmatrix}$$
$$+ \frac{1}{Y_1 - Y_2}\left(A\begin{pmatrix} X_1+X_2 \\ Y_1 \end{pmatrix} - A\begin{pmatrix} X_1+X_2 \\ Y_2 \end{pmatrix}\right),$$
$$A\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} \cdot A\begin{pmatrix} X_2, X_3 \\ Y_2, Y_3 \end{pmatrix} = A\begin{pmatrix} X_1+X_2, X_2, X_3 \\ Y_1, Y_2, Y_3 \end{pmatrix} + A\begin{pmatrix} X_1+X_2, X_1+X_3, X_3 \\ Y_2, Y_1, Y_3 \end{pmatrix}$$
$$+ A\begin{pmatrix} X_1+X_2, X_1+X_3, X_1 \\ Y_2, Y_3, Y_1 \end{pmatrix} + \frac{1}{Y_1 - Y_2}\left(A\begin{pmatrix} X_1+X_2, X_3 \\ Y_1, Y_3 \end{pmatrix} - A\begin{pmatrix} X_1+X_2, X_3 \\ Y_2, Y_3 \end{pmatrix}\right)$$
$$+ \frac{1}{Y_1 - Y_3}\left(A\begin{pmatrix} X_1+X_2, X_1+X_3 \\ Y_2, Y_1 \end{pmatrix} - A\begin{pmatrix} X_1+X_2, X_1+X_3 \\ Y_2, Y_3 \end{pmatrix}\right).$$

Finally, we want to relate the previously introduced sets $\mathrm{GBARI}_{q\text{-as},\tau}$ and $\mathrm{GBARI}_{q\text{-is},\tau}$ to the following sets.

Definition 2.73. Define the subsets

$$\mathrm{GBARI}_{\mathrm{as,swap}} = \{A \in \mathrm{GBARI} \mid A \text{ symmetral and swap invariant}\},$$
$$\mathrm{GBARI}_{\mathrm{is,swap}} = \{A \in \mathrm{GBARI} \mid A \text{ symmetril and swap invariant}\}.$$

Note that by Theorem 2.46, the bimould $\mathfrak{G}$ of the generating series of the combinatorial bi-multiple Eisenstein series is contained in $\mathrm{GBARI}_{\mathrm{is,swap}}^{\mathrm{pow},\mathcal{Z}_q}$.

Definition 2.74. For a bimould $A \in \mathrm{BIMU}$, define for each $d \geq 1$

$$A^{\#_Y}\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = A\begin{pmatrix} X_1,\dots,X_d \\ Y_1, Y_1+Y_2,\dots,Y_1+\dots+Y_d \end{pmatrix}.$$

Theorem 2.75. *The map $\#_Y$ restricts to bijections*

$$\#_Y : \mathrm{GBARI}_{q\text{-as},\tau} \to \mathrm{GBARI}_{\mathrm{as,swap}}, \qquad \#_Y : \mathrm{GBARI}_{q\text{-is},\tau} \to \mathrm{GBARI}_{\mathrm{is,swap}}.$$

Note that τ-invariance induces relations on the coefficients, which are much easier to handle than the relations induced by swap invariance (cf (2.65.1) and Example C.11). Thus, it seems convenient to consider the sets $\mathrm{GBARI}_{q\text{-as},\tau}$ and $\mathrm{GBARI}_{q\text{-is},\tau}$ instead of $\mathrm{GBARI}_{\mathrm{as,swap}}$ and $\mathrm{GBARI}_{\mathrm{is,swap}}$.

Proof. Let $A \in \mathrm{GBARI}_{q\text{-as},\tau}$. First, we show that $A^{\#_Y}$ is symmetral. For all $d, d' \geq 1$ denote by $\sqcup\!\sqcup(d,d')$ the set of all permutations $\sigma \in S_{d+d'}$ satisfying $\sigma(1) < \cdots < \sigma(d)$, $\sigma(d+1) < \cdots < \sigma(d+d')$. Moreover, write $\underline{Y_i} = Y_1 + \cdots + Y_i$ for $1 \leq i \leq d$ and $\underline{Y_{d+j}} = Y_{d+1} + \cdots + Y_{d+j}$ for $1 \leq j \leq d'$. Then the q-symmetrality of A implies by Proposition A.78 (i)

$$
\begin{aligned}
&A_d^{\#_Y}\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} A_{d'}^{\#_Y}\binom{X_{d+1},\dots,X_{d+d'}}{Y_{d+1},\dots,Y_{d+d'}} \qquad (2.75.1)\\
&\qquad = \sum_{\sigma\in\sqcup\!\sqcup(d,d')} A_{d+d'}\left(\begin{matrix} X_{\sigma^{-1}(1)},\dots,X_{\sigma^{-1}(d+d')} \\ \underline{Y_{\sigma^{-1}(1)}}+\underline{Y_{\sigma_\mu^{-1}(1)}},\dots,\underline{Y_{\sigma^{-1}(d+d')}}+\underline{Y_{\sigma_\mu^{-1}(d+d')}}\end{matrix}\right),
\end{aligned}
$$

where we set $\sigma_\mu^{-1}(k) = \begin{cases} \sigma^{-1}\big(\max\{n \mid \sigma^{-1}(n) > d, n < k\}\big), & 1 \leq \sigma^{-1}(k) \leq d, \\ \sigma^{-1}\big(\max\{n \mid \sigma^{-1}(n) \leq d,\ n < k\}\big), & d+1 \leq \sigma^{-1}(k) \leq d+d' \end{cases}$ and $Y_{\sigma_\mu^{-1}(k)} = 0$ if such a number n does not exists. Applying the inverse

$$
\#_Y^{-1} : M\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} \mapsto M\binom{X_1,X_2,\dots,X_d}{Y_1,Y_2-Y_1,\dots,Y_d-Y_{d-1}}
$$

to any terms in the above sum, we get

$$
A_{d+d'}^{\#_Y^{-1}}\left(\begin{matrix} X_{\sigma^{-1}(1)},\dots,X_{\sigma^{-1}(d+d')} \\ \underline{Y_{\sigma^{-1}(1)}}+\underline{Y_{\sigma_\mu^{-1}(1)}},\dots,\underline{Y_{\sigma^{-1}(d+d')}}+\underline{Y_{\sigma_\mu^{-1}(d+d')}}\end{matrix}\right) = A_{d+d'}\binom{X_{\sigma^{-1}(1)},\dots,X_{\sigma^{-1}(d+d')}}{Y_{\sigma^{-1}(1)},\dots,Y_{\sigma^{-1}(d+d')}}. \qquad (2.75.2)
$$

To obtain this formula observe that for every $k = 1,\dots,d+d'$ the predecessor of the entry $\underline{Y_{\sigma^{-1}(k)}} + \underline{Y_{\sigma_\mu^{-1}(k)}}$ in the bi-index is given by $\underline{Y_{\sigma^{-1}(k)-1}} + \underline{Y_{\sigma_\mu^{-1}(k)}}$ (where $\underline{Y_{\sigma^{-1}(k)-1}} := 0$ if $k \in \{1, d+1\}$) and, moreover, we have $\underline{Y_n} - \underline{Y_{n-1}} = Y_n$. Combining the equations (2.75.1) and (2.75.2), we get

$$
A_d^{\#_Y}\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} A_{d'}^{\#_Y}\binom{X_{d+1},\dots,X_{d+d'}}{Y_{d+1},\dots,Y_{d+d'}} = \sum_{\sigma\in\sqcup\!\sqcup(d,d')} A_{d+d'}^{\#_Y}\binom{X_{\sigma^{-1}(1)},\dots,X_{\sigma^{-1}(d+d')}}{Y_{\sigma^{-1}(1)},\dots,Y_{\sigma^{-1}(d+d')}}.
$$

From Corollary A.76 we deduce that $A^{\#_Y}$ is symmetral. The proof that $A^{\#_Y}$ is symmetril for all $A \in \mathrm{GBARI}_{q\text{-is},\tau}$ is similar. Just observe that for every entry $\binom{X_j}{\underline{Y_j}+\underline{Y_{j'}}}$ coming from the third line in the recursive expression of $*_q$ given in Proposition A.78 (ii), the predecessor of the lower row is given by $\underline{Y_{j-1}}+\underline{Y_{j'-1}}$ (with $\underline{Y_{1-1}} = \underline{Y_{d+1-1}} = 0$). Moreover, we compute straight-forward

$$
\begin{aligned}
\tau(A)^{\#_Y}\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} &= \tau(A)\binom{X_1,X_2,\dots,X_d}{Y_1,Y_1+Y_2,\dots,Y_1+\cdots+Y_d} \\
&= A\binom{Y_1+\cdots+Y_d, Y_1+\cdots+Y_{d-1},\dots,Y_1}{X_d,X_{d-1},\dots,X_1} \\
&= A^{\#_Y}\binom{Y_1+\cdots+Y_d, Y_1+\cdots+Y_{d-1},\dots,Y_1}{X_d,X_{d-1}-X_d,\dots,X_1-X_2} \\
&= \mathrm{swap}\left(A^{\#_Y}\right)\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}.
\end{aligned}
$$

In particular, a bimould A is τ-invariant if and only if $A^{\#_Y}$ is swap invariant. □

Theorem 2.75 enables us to prove the following proposition from the previous subsection.

Proposition 2.55. The bimould $\mathfrak{B}$ is q-symmetril and τ-invariant.

Proof. Observe that we have by definition $\mathfrak{B} = \mathfrak{G}^{\#_Y^{-1}}$. Since $\mathfrak{G}$ is contained in $\mathrm{GBARI}_{\mathrm{is,swap}}^{\mathrm{pow},\mathcal{Z}_q}$ (Theorem 2.46) and there is a bijection $\#_Y : \mathrm{GBARI}_{q\text{-is},\tau}^{\mathrm{pow},\mathcal{Z}_q} \to \mathrm{GBARI}_{\mathrm{is,swap}}^{\mathrm{pow},\mathcal{Z}_q}$ (Theorem 2.75),we deduce that the bimould $\mathfrak{B}$ is q-symmetril and τ-invariant. □

3 The q-Ihara bracket

G. Racinet introduced in [Rac00] the twisted Magnus[3] affine group scheme MT and the twisted Magnus Lie algebra $\mathfrak{mt}$ and proved that the double shuffle Lie algebra $\mathfrak{dm}_0$ and its corresponding affine group scheme DM_0 embed in there (cf Theorem B.30). In this section we first recall the results obtained in [Rac00] for the twisted Magnus affine group scheme and Lie algebra. Then we will introduce a q-analog of this Lie algebra, which can be seen as a generalization of $\mathfrak{mt}$, and explain what is known towards the corresponding group multiplication.

3.1 Twisted Magnus affine group scheme MT and the Lie algebra $\mathfrak{mt}$

Let $\mathcal{A}$ be an alphabet and $(\mathbb{Q}\langle\mathcal{A}\rangle, \cdot)$ the free non-commutative algebra over $\mathcal{A}$ equipped with the concatenation product. The empty word is denoted by $\mathbf{1}$. Define the degree of each word in $\mathbb{Q}\langle\mathcal{A}\rangle$ to be the number of its letters, this defines a grading on the algebra $(\mathbb{Q}\langle\mathcal{A}\rangle, \cdot)$. For each commutative $\mathbb{Q}$-algebra R with unit, denote by $R\langle\langle\mathcal{A}\rangle\rangle$ the completion of $R\langle\mathcal{A}\rangle = \mathbb{Q}\langle\mathcal{A}\rangle \otimes R$ with respect to this grading (in the sense of Proposition A.45).

Definition 3.1. For each commutative $\mathbb{Q}$-algebra R with unit, denote

$$\mathsf{M}(R) = \{f \in R\langle\langle\mathcal{A}\rangle\rangle \mid (f \mid \mathbf{1}) = 1\},$$

where $(f \mid \mathbf{1})$ denotes the coefficient of f in $\mathbf{1}$. Then

$$\mathsf{M} : \mathbb{Q}\text{-Alg} \to \text{Groups}, \;\; R \mapsto (\mathsf{M}(R), \cdot)$$

is called the Magnus affine group scheme.

It is obvious that the concatenation product $\cdot$ is associative and possesses an identity element in $\mathsf{M}(R)$. Moreover one easily verifies that the inverse of an element $G = \mathbf{1} + g$ in $\mathsf{M}(R)$ with respect to the concatenation product is given by

$$G^{-1} = \mathbf{1} + \sum_{n\geq 1} (-1)^n g^n \in \mathsf{M}(R).$$

Thus, $(\mathsf{M}(R), \cdot)$ is indeed a group.

Definition 3.2. For each commutative $\mathbb{Q}$-algebra R with unit, define

$$\mathfrak{m}(R) = \{f \in R\langle\mathcal{A}\rangle \mid (f \mid \mathbf{1}) = 0\}.$$

Then $(\mathfrak{m}(R), [-,-])$ is called the Magnus Lie algebra, where $[-,-]$ denotes the usual commutator bracket on $(R\langle\mathcal{A}\rangle, \cdot)$.

One derives immediately from Definition A.88 that the Lie algebra functor to the Magnus affine group scheme M is given by

$$\widehat{\mathfrak{m}} : \mathbb{Q}\text{-Alg} \to \text{Lie-Alg} \quad R \mapsto (\widehat{\mathfrak{m}}(R), [-,-]),$$

where $\widehat{\mathfrak{m}}(R)$ denotes the completion of $\mathfrak{m}(R)$ with respect to the grading on $R\langle\mathcal{A}\rangle$ defined above. In Example A.96 it is explained in detail, how to derive the commutator bracket from the concatenation product on M.

Now we will restrict to a specific alphabet consisting of two letters and consider a twisted

[3] In [Rac00] the affine group scheme is called "Magnus tordu"

version of the Magnus affine group scheme and Lie algebra. Precisely, consider the alphabet $\mathcal{X} = \{x_0, x_1\}$ and denote by $\mathbb{Q}\langle\mathcal{X}\rangle$ the free non-commutative algebra over $\mathcal{X}$. Define the weight of a word in $\mathbb{Q}\langle\mathcal{X}\rangle$ to be the number of its letters. For each commutative $\mathbb{Q}$-algebra R with unit, we denote by $R\langle\langle\mathcal{X}\rangle\rangle$ the completion of $R\langle\mathcal{X}\rangle = \mathbb{Q}\langle\mathcal{X}\rangle \otimes R$ with respect to the weight. In other words, the space $R\langle\langle\mathcal{X}\rangle\rangle$ consists of formal non-commutative power series in the letters x_0, x_1 with coefficients in R.

Definition 3.3. For any commutative $\mathbb{Q}$-algebra R with unit, define

$$\mathsf{MT}(R) = \{f \in R\langle\langle\mathcal{X}\rangle\rangle \mid (f \mid \mathbf{1}) = 1\}.$$

For $G \in \mathsf{MT}(R)$, define the algebra automorphism (with respect to concatenation)

$$\kappa_G : R\langle\langle\mathcal{X}\rangle\rangle \to R\langle\langle\mathcal{X}\rangle\rangle$$

by

$$\kappa_G(\mathbf{1}) = \mathbf{1}, \qquad \kappa_G(x_0) = x_0, \qquad \kappa_G(x_1) = G^{-1}x_1G.$$

Then set

$$G \circledast H = G\kappa_G(H), \qquad G, H \in \mathsf{MT}(R).$$

Note that the product $\circledast$ only differs from the usual concatenation product by the twist in x_1 (in the definition of κ).

Proposition 3.4. *([Rac00, II, Proposition 2.4]) For each commutative $\mathbb{Q}$-algebra R with unit, the pair $(\mathsf{MT}(R), \circledast)$ is a group.*

Proof. Evidently, the multiplication $\circledast$ preserves the set $\mathsf{MT}(R)$. Observe that the identity element for the multiplication $\circledast$ is given by $\mathbf{1}$, since $\kappa_G(\mathbf{1}) = \mathbf{1}$ and $\kappa_{\mathbf{1}}(G) = G$ for each $G \in \mathsf{MT}(R)$. To prove the associativity of $\circledast$, first compute for $G_1, G_2 \in \mathsf{MT}(R)$ that

$$\begin{aligned}
(\kappa_{G_1} \circ \kappa_{G_2})(x_0) &= x_0,\\
(\kappa_{G_1} \circ \kappa_{G_2})(x_1) &= \kappa_{G_1}(G_2^{-1}x_1G_2) = \kappa_{G_1}(G_2^{-1})G_1^{-1}x_1G_1\kappa_{G_1}(G_2)\\
&= \Big(G_1\kappa_{G_1}(G_2)\Big)^{-1}x_1\Big(G_1\kappa_{G_1}(G_2)\Big) = (G_1 \circledast G_2)^{-1}x_1(G_1 \circledast G_2)\\
&= \kappa_{G_1 \circledast G_2}(x_1).
\end{aligned}$$

Thus, one has $\kappa_{G_1} \circ \kappa_{G_2} = \kappa_{G_1 \circledast G_2}$ and can deduce for $G_1, G_2, H \in \mathsf{MT}(R)$

$$\begin{aligned}
G_1 \circledast (G_2 \circledast H) &= G_1 \circledast (G_2\kappa_{G_2}(H)) = G_1\kappa_{G_1}(G_2)\kappa_{G_1}(\kappa_{G_2}(H)) = G_1\kappa_{G_1}(G_2)\kappa_{G_1 \circledast G_2}(H)\\
&= (G_1 \circledast G_2)\kappa_{G_1 \circledast G_2}(H) = (G_1 \circledast G_2) \circledast H.
\end{aligned}$$

Finally, it has to be shown that any $G \in \mathsf{MT}(R)$ has an inverse. For $H = \kappa_G^{-1}(G^{-1}) \in \mathsf{MT}(R)$ one computes

$$G \circledast H = G\kappa_G(H) = G\kappa_G(\kappa_G^{-1}(G^{-1})) = GG^{-1} = \mathbf{1}.$$

By group theory, it is enough to show that G has a right inverse. □

Theorem 3.5. *The functor $\mathsf{MT} : \mathbb{Q}\text{-Alg} \to \text{Groups},\ R \mapsto (\mathsf{MT}(R), \circledast)$ is a pro-unipotent affine group scheme.*

We will refer to MT as the twisted Magnus affine group scheme.

Proof. MT is an affine scheme represented by the algebra $\mathbb{Q}[(z_w)_{w\in\mathcal{X}^*}]\big/(z_{\mathbf{1}}-1)$ and thus by Proposition 3.4 an affine group scheme. For the pro-unipotence, we refer to [Rac00, Section II.2]. □

Definition 3.6. For each commutative $\mathbb{Q}$-algebra R with unit, define

$$\mathfrak{mt}(R) = \{f \in R\langle\mathcal{X}\rangle \mid (f \mid \mathbf{1}) = 0.\}$$

Moreover, set $\mathfrak{mt} = \mathfrak{mt}(\mathbb{Q})$.

It is obvious from Definition A.88 that

$$\widehat{\mathfrak{mt}} : \mathbb{Q}\text{-Alg} \to \text{Lie-Alg},\ R \mapsto \widehat{\mathfrak{mt}}(R)$$

is the Lie algebra functor to the affine group scheme MT, where $\widehat{\mathfrak{mt}}(R)$ is the completion of $\mathfrak{mt}(R)$ with respect to the weight. In particular, the space $\mathfrak{mt}(R)$ admits a Lie algebra structure, which can be derived from the group multiplication $\circledast$ on MT.

Theorem 3.7. *Let R be a commutative $\mathbb{Q}$-algebra with unit. Then the space $\mathfrak{mt}(R)$ is a Lie algebra equipped with the Lie bracket*

$$\{f, g\} = d_f(g) - d_g(f) + [f, g], \qquad f, g \in \mathfrak{mt}(R),$$

where $d_f : R\langle\mathcal{X}\rangle \to R\langle\mathcal{X}\rangle$ is the derivation defined by $d_f(\mathbf{1}) = 0$, $d_f(x_0) = 0$ and $d_f(x_1) = [x_1, f]$.

We call $(\mathfrak{mt}(R), \{-,-\})$ the twisted Magnus Lie algebra and the Lie bracket $\{-,-\}$ the Ihara bracket.

Proof. For any $G \in \mathsf{MT}(R)$, consider the endomorphism

$$\sigma(G) : R\langle\langle\mathcal{X}\rangle\rangle \to R\langle\langle\mathcal{X}\rangle\rangle,\ H \mapsto G \circledast H.$$

Let $R[\varepsilon]$ be the algebra of dual numbers with $\varepsilon^2 = 0$. For $f \in \widehat{\mathfrak{mt}}(R)$, define the endomorphism $s_f : R\langle\langle\mathcal{X}\rangle\rangle \to R\langle\langle\mathcal{X}\rangle\rangle$ by

$$\sigma(\mathbf{1} + \varepsilon f) = \mathrm{id} + \varepsilon s_f.$$

Let $\{-,-\}$ be the corresponding Lie bracket to $\circledast$, then we have

$$s_{\{f,g\}} = [s_f, s_g], \qquad f, g \in \widehat{\mathfrak{mt}}(R). \tag{3.7.1}$$

Moreover, one computes for $f \in \widehat{\mathfrak{mt}}(R)$

$$\mathbf{1} + \varepsilon f = \sigma(\mathbf{1} + \varepsilon f)(\mathbf{1}) = (\mathrm{id} + \varepsilon s_f)(\mathbf{1}) = \mathbf{1} + \varepsilon s_f(\mathbf{1})$$

and thus $s_f(\mathbf{1}) = f$. Combining this with (3.7.1) leads to

$$\{f, g\} = s_f(g) - s_g(f), \qquad f, g \in \widehat{\mathfrak{mt}}(R). \tag{3.7.2}$$

Furthermore, for $f \in \widehat{\mathfrak{mt}}(R)$ define the endomorphism $d_f : R\langle\langle\mathcal{X}\rangle\rangle \to R\langle\langle\mathcal{X}\rangle\rangle$ by

$$\kappa_{\mathbf{1}+\varepsilon f} = \mathrm{id} + \varepsilon d_f.$$

Then one calculates for $f \in \widehat{\mathfrak{mt}}(R)$ and $u, v \in R\langle\langle\mathcal{X}\rangle\rangle$

$$\kappa_{\mathbf{1}+\varepsilon f}(uv) = \kappa_{\mathbf{1}+\varepsilon f}(u)\kappa_{\mathbf{1}+\varepsilon f}(v) = (u + \varepsilon d_f(u))(v + \varepsilon d_f(v)) = uv + \varepsilon(u d_f(v) + d_f(u)v).$$

So d_f is a derivation for the concatenation product and it suffices to obtain an explicit formula on the generators. One has

$$\kappa_{\mathbf{1}+\varepsilon f}(x_0) = x_0 + \varepsilon \cdot 0,$$
$$\kappa_{\mathbf{1}+\varepsilon f}(x_1) = (\mathbf{1}+\varepsilon f)^{-1} x_1 (\mathbf{1}+\varepsilon f) = (\mathbf{1}-\varepsilon f) x_1 (\mathbf{1}+\varepsilon f) = x_1 + \varepsilon(x_1 f - f x_1).$$

Therefore, d_f is the derivation determined by $d_f(x_0) = 0$ and $d_f(x_1) = [x_1, f]$. Finally, compute for $f \in \widehat{\mathfrak{mt}}(R)$ and $w \in R\langle\langle \mathcal{X} \rangle\rangle$

$$\sigma(\mathbf{1}+\varepsilon f)(w) = (\mathbf{1}+\varepsilon f)\kappa_{\mathbf{1}+\varepsilon f}(w) = (\mathbf{1}+\varepsilon f)(w + \varepsilon d_f(w)) = w + \varepsilon(d_f(w) + f w)$$

and hence

$$s_f(w) = d_f(w) + f w.$$

From (3.7.2) one obtains then that the Lie bracket on $\widehat{\mathfrak{mt}}(R)$ (and hence also on $\mathfrak{mt}(R)$) is given by

$$\{f, g\} = d_f(g) + fg - d_g(f) - gf.$$

□

3.2 The q-twisted Magnus Lie algebra $\mathfrak{mq}$

After reviewing the results in [Rac00] on the twisted Magnus affine group scheme and Lie algebra, we will introduce now the q-twisted Magnus Lie algebra. In particular, our main result will be a generalization of Theorem 3.7.

Consider the alphabet $\mathcal{B} = \{b_0, b_1, b_2, \ldots\}$ and denote by $\mathbb{Q}\langle\mathcal{B}\rangle$ the free algebra over $\mathcal{B}$. Moreover, for a word in $\mathbb{Q}\langle\mathcal{B}\rangle$ define the weight and depth by

$$\begin{aligned}\mathrm{wt}(b_0^{m_0} b_{k_1} b_0^{m_1} \ldots b_{k_d} b_0^{m_d}) &= k_1 + \cdots + k_d + m_0 + \cdots + m_d,\\ \mathrm{dep}(b_0^{m_0} b_{k_1} b_0^{m_1} \ldots b_{k_d} b_0^{m_d}) &= d,\end{aligned}$$

where $k_1, \ldots, k_d \geq 1,\ m_0, \ldots, m_d \geq 0$.

Definition 3.8. We define the $\mathbb{Q}$-linear map ∂_i on $\mathbb{Q}\langle\mathcal{B}\rangle$ by

$$\partial_i(b_0^{m_0} b_{k_1} b_0^{m_1} \ldots b_{k_d} b_0^{m_d}) = b_0^{m_0} b_{k_1} b_0^{m_1} \ldots b_{k_{i-1}} b_0^{m_{i-1}} b_{k_i+1} b_0^{m_i} b_{k_{i+1}} b_0^{m_{i+1}} \ldots b_{k_d} b_0^{m_d}$$

if $1 \leq i \leq d$ and $\partial_i(b_0^{m_0} b_{k_1} b_0^{m_1} \ldots b_{k_d} b_0^{m_d}) = 0$ else.

For a word $w = b_0^{m_0} b_{k_1} b_0^{m_1} \ldots b_{k_d} b_0^{m_d}$ (where $k_1, \ldots, k_d \geq 1,\ m_0, \ldots, m_d \geq 0$) and a positive integer $1 \leq j \leq d$, we set then

$$\delta_j(w) = \prod_{\substack{i=1\\ i\neq j}}^{d} (\partial_i - \partial_j)^{k_i - 1} (b_0^{m_0} b_1 b_0^{m_1} \ldots b_1 b_0^{m_{j-1}} b_{k_j} b_0^{m_j} b_1 b_0^{m_{j+1}} \ldots b_1 b_0^{m_d})$$

and extend this definition by $\mathbb{Q}$-linearity.

Example 3.9. For $k, a \geq 1$, we compute

$$\begin{aligned}\delta_2(b_k b_a) &= (\partial_1 - \partial_2)^{k-1}(b_1 b_a) = \sum_{l=0}^{k-1} (-1)^l \binom{k-1}{l} b_{k-l} b_{a+l},\\ \delta_1(b_a b_k) &= (\partial_2 - \partial_1)^{k-1}(b_a b_1) = \sum_{l=0}^{k-1} (-1)^l \binom{k-1}{l} b_{a+l} b_{k-l}.\end{aligned}$$

Thus we deduce

$$\delta_2(b_k b_a) - \delta_1(b_a b_k) = \sum_{l=0}^{k-1} (-1)^l \binom{k-1}{l} [b_{k-l}, b_{a+l}].$$

Definition 3.10. For any word $w = b_0^{m_0} b_{k_1} b_0^{m_1} \ldots b_{k_d} b_0^{m_d}$ in $\mathbb{Q}\langle\mathcal{B}\rangle$ (where $k_1, \ldots, k_d \geq 1,\ m_0, \ldots, m_d \geq 0$) and $r \geq 1$, $a < k_j$, we set

$$\begin{aligned}\mathrm{lc}_j^{(a,0)}(w) &= w,\\ \mathrm{lc}_j^{(a,r)}(w) &= \sum_{\substack{j_1+\cdots+j_{r+1}=k_j-a\\ j_1,\ldots,j_{r+1}\geq 1}} b_{a+j_1} b_{j_2} \ldots b_{j_r} b_0^{m_0} b_{k_1} b_0^{m_1} \ldots b_{k_{j-1}} b_0^{m_{j-1}} b_{j_{r+1}} b_0^{m_j} b_{k_{j+1}} b_0^{m_{j+1}} \ldots b_{k_d} b_0^{m_d}\end{aligned}$$

and extend this definition by $\mathbb{Q}$-linearity.

Example 3.11. We have

$$\begin{aligned}\mathrm{lc}_2^{(6,2)}(b_{13} b_{11}) &= \sum_{\substack{j_1+j_2+j_3=5\\ j_1,j_2,j_3\geq 1}} b_{6+j_1} b_{j_2} b_{13} b_{j_3}\\ &= b_9 b_1 b_{13} b_1 + b_7 b_3 b_{13} b_1 + b_7 b_1 b_{13} b_3 + b_8 b_2 b_{13} b_1 + b_8 b_1 b_{13} b_2 + b_7 b_2 b_{13} b_2.\end{aligned}$$

Definition 3.12. For a given word $w = b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}$, we define the derivation d_w^q on $(\mathbb{Q}\langle\mathcal{B}\rangle, \cdot)$ by its values on the generators

$$\begin{aligned}
d_w^q(\mathbf{1}) &= d_w^q(b_0) = 0,\\
d_w^q(b_a) &= \sum_{r=0}^{k_1+\dots+k_d-d} (-1)^r \Big(\mathrm{lc}_{d+1}^{(a-1,r)} \circ \delta_{d+1}(wb_a) - \mathrm{lc}_1^{(a-1,r)} \circ \delta_1(b_a w) \Big), \quad a \geq 1.
\end{aligned}$$

Moreover, we set for a word $w = b_0^m$ in $\mathbb{Q}\langle\mathcal{B}\rangle$ of depth 0

$$d_w^q(\mathbf{1}) = d_w^q(b_0) = 0, \qquad d_w^q(b_a) = [w, b_a], \quad a \geq 1.$$

As before, extend this definition by $\mathbb{Q}$-linearity.

Lemma 3.13. *We have for d_w^q, where $w = b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}$, the explicit formula*

$$\begin{aligned}
&d_w^q(b_a) = [w, b_a]\\
&+ \sum_{\substack{l_1=0 \\ (l_1,\dots,l_d)\neq(0,\dots,0)}}^{k_1-1} \cdots \sum_{l_d=0}^{k_d-1} \binom{k_1-1}{l_1} \cdots \binom{k_d-1}{l_d} (-1)^{l_1+\dots+l_d}\\
&\cdot \Bigg(\Big[b_0^{m_0} b_{k_1-l_1} b_0^{m_1} \dots b_{k_d-l_d} b_0^{m_d}, b_{a+l_1+\dots+l_d} \Big]\\
&+ \sum_{r=1}^{k_1+\dots+k_d-d} (-1)^r \sum_{\substack{j_1+\dots+j_{r+1}=l_1+\dots+l_d+1 \\ j_1,\dots,j_{r+1}\geq 1}} b_{a+j_1-1} b_{j_2} \dots b_{j_r} \Big[b_0^{m_0} b_{k_1-l_1} b_0^{m_1} \dots b_{k_d-l_d} b_0^{m_d}, b_{j_{r+1}} \Big] \Bigg)
\end{aligned}$$

with $a \geq 1$.

Proof. This follows straight-forwardly from applying the definitions. □

Note that for $k_1 = \dots = k_d = 1$ all sums in Lemma 3.13 vanish. So the first term $[w, b_a]$ in the above expression of $d_w^q(b_a)$ should be seen as the part from the Ihara bracket (cf Theorem 3.7). The terms in the third row extend the Ihara bracket part to the whole algebra $\mathbb{Q}\langle\mathcal{B}\rangle$, and the terms in the fourth row handle the non depth-graded parts.

Example 3.14. One computes

$$\begin{aligned}
d_{b_2b_0-b_0b_2}^q(b_1) &= [b_2b_0 - b_0b_2, b_1] - [b_1b_0 - b_0b_1, b_2] + b_1[b_1b_0 - b_0b_1, b_1],\\
d_{b_1}^q(b_2b_0 - b_0b_2) &= [b_1, b_2]b_0 - b_0[b_1, b_2],
\end{aligned}$$

Lemma 3.15. *(i) If $w \in \mathbb{Q}\langle b_0, b_1\rangle$, then d_w^q is a special derivation (as in Theorem 3.7)*

$$d_w^q(b_0) = 0, \qquad d_w^q(b_a) = [w, b_a] \quad \text{for } a \geq 1.$$

(ii) The assignment $(w, v) \mapsto d_w^q(v)$ is homogeneous for the weight, i.e., one has

$$\mathrm{wt}\left(d_w^q(v)\right) = \mathrm{wt}(w) + \mathrm{wt}(v).$$

Proof. (i) follows immediately from $\delta_j(w_1 b_a w_2) = w_1 b_a w_2$ for $w_1, w_2 \in \mathbb{Q}\langle b_0, b_1\rangle$, $\mathrm{dep}(w_1) = j-1$ and $\mathrm{lc}_j^{(a,0)} = \mathrm{id}$. (ii) can be read of from Lemma 3.13. □

Note that $(w, v) \mapsto d_w^q(v)$ is not homogeneous for the depth on $\mathbb{Q}\langle\mathcal{B}\rangle$, the last line in the definition of d_w^q produces terms of depth $> \mathrm{dep}(v) + \mathrm{dep}(w)$.

The following definition is the main definition of this section, observe its similarities to Theorem 3.7.

Definition 3.16. For $f, g \in \mathbb{Q}\langle\mathcal{B}\rangle$, we define the q-Ihara bracket as

$$\{f, g\}_q = d_f^q(g) - d_g^q(f) - [f, g].$$

Moreover, for $f, g \in \mathbb{Q}\langle\mathcal{B}\rangle$ the pre-Lie multiplication of the q-Ihara bracket is given by

$$s_f^q(g) = d_f^q(g) + gf.$$

Thus, we also have

$$\{f, g\}_q = s_f^q(g) - s_g^q(f).$$

Example 3.17. With the results in Example 3.14, one computes

$$\begin{aligned}\{b_2b_0 - b_0b_2, b_1\}_q = & -[b_1b_0 - b_0b_1, b_2] + b_1[b_1b_0 - b_0b_1, b_1] - [b_1, b_2]b_0 + b_0[b_1, b_2] \\ = & -b_1b_0b_2 + 2b_0b_1b_2 + 2b_2b_1b_0 - b_2b_0b_1 - b_1b_2b_0 - b_0b_2b_1 \\ & + 2b_1^2b_0b_1 - b_1b_0b_1^2 - b_1^3b_0\end{aligned}$$

One of the main results of this thesis is that the q-Ihara bracket is indeed a Lie bracket, so it satisfies anti-symmetry and Jacobi's identity. In particular, we will obtain a Lie algebra $(\mathfrak{mq}, \{-,-\}_q)$ (Theorem 3.20), which should be seen as a q-analog of the twisted Magnus Lie algebra $(\mathfrak{mt}, \{-,-\})$ (Theorem 3.7). To obtain these results, we need the following.

Key Lemma 3.18. *For all $f, g \in \mathbb{Q}\langle\mathcal{B}\rangle$, the following equality holds*

$$d^q_{\{f,g\}_q} = [d_f^q, d_g^q],$$

where $[-,-]$ denotes the usual commutator bracket.

The proof is given in Subsection 3.3.

As an analog of the twisted Magnus Lie algebra $\mathfrak{mt}$ (Definition 3.6), define the following.

Definition 3.19. Let $\mathfrak{mq}$ be the subspace of $\mathbb{Q}\langle\mathcal{B}\rangle$ given by

$$\mathfrak{mq} = \{f \in \mathbb{Q}\langle\mathcal{B}\rangle \mid (f \mid \mathbf{1}) = 0\}.$$

Theorem 3.20. *The pair $(\mathfrak{mq}, \{-,-\}_q)$ is a Lie algebra.*

We will refer to this Lie algebra as the q-twisted Magnus Lie algebra[4].

Proof. From Lemma 3.15 (ii) we immediately obtain that the q-Ihara bracket $\{-,-\}_q$ preserves the space $\mathfrak{mq}$. It is clear from Definition 3.16 that the q-Ihara bracket is anti-symmetric. Thus we only need to check Jacobi's identity (see Definition A.9). We compute for all $f, g, h \in \mathbb{Q}\langle\mathcal{B}\rangle$

$$\begin{aligned}&\{f, \{g, h\}_q\}_q + \{g, \{h, f\}_q\}_q + \{h, \{f, g\}_q\}_q \\ &= d_f^q(d_g^q(h)) - d_f^q(d_h^q(g)) - d_f^q([g, h]) - d^q_{\{g,h\}_q}(f) - [f, d_g^q(h)] + [f, d_h^q(g)] + [f, [g, h]] \\ &+ d_g^q(d_h^q(f)) - d_g^q(d_f^q(h)) - d_g^q([h, f]) - d^q_{\{h,f\}_q}(g) - [g, d_h^q(f)] + [g, d_f^q(h)] + [g, [f, h]] \\ &+ d_h^q(d_f^q(g)) - d_h^q(d_g^q(f)) - d_h^q([f, g]) - d^q_{\{f,g\}_q}(h) - [h, d_f^q(g)] + [h, d_g^q(f)] + [h, [f, g]] \\ &= [d_f^q, d_g^q](h) + [d_g^q, d_h^q](f) + [d_h^q, d_f^q](g) - d^q_{\{g,h\}_q}(f) - d^q_{\{h,f\}_q}(g) - d^q_{\{f,g\}_q}(g) \\ &= 0.\end{aligned}$$

[4] After the submission of this thesis, the author was informed by D. Manchon that the q-twisted Magnus Lie algebra has a post-Lie structure as introduced in [ELM15]

The second equality follows from simple cancellation and Jacobi's identity applied to the commutator bracket, the third equality is obtained from Key Lemma 3.18. □

The q-twisted Magnus Lie algebra $(\mathfrak{mq}, \{-,-\}_q)$ is a generalization of the twisted Magnus algebra $(\mathfrak{mt}, \{-,-\})$ (Theorem 3.7), precisely the following holds.

Proposition 3.21. *There is an embedding of Lie algebras*

$$\theta_{\mathcal{X}}^{-} : (\mathfrak{mt}, \{-,-\}) \hookrightarrow (\mathfrak{mq}, \{-,-\}_q),$$
$$x_{s_1} \dots x_{s_l} \mapsto -b_{s_1} \dots b_{s_l}$$

Proof. Let $f, g \in \mathfrak{mt}$. Recall that the derivation d_f in the Ihara bracket is given by $d_f(x_0) = x_0,\ d_f(x_1) = [x_1, f]$. Thus, Lemma 3.15 (i) implies that

$$\theta_{\mathcal{X}}^{-}(d_f(g)) = d^q_{\theta_{\mathcal{X}}^{-}(f)}(\theta_{\mathcal{X}}^{-}(g))$$

and therefore one computes

$$\begin{aligned}
\theta_{\mathcal{X}}^{-}(\{f,g\}) &= \theta_{\mathcal{X}}^{-}(d_f(g)) - \theta_{\mathcal{X}}^{-}(d_g(f)) + \theta_{\mathcal{X}}^{-}([f,g]) \\
&= d^q_{\theta_{\mathcal{X}}^{-}(f)}(\theta_{\mathcal{X}}^{-}(g)) - d^q_{\theta_{\mathcal{X}}^{-}(g)}(\theta_{\mathcal{X}}^{-}(f)) - [\theta_{\mathcal{X}}^{-}(f), \theta_{\mathcal{X}}^{-}(g)] \\
&= \{\theta_{\mathcal{X}}^{-}(f), \theta_{\mathcal{X}}^{-}(g)\}_q.
\end{aligned}$$

□

Remark 3.22. In Section 4 we will embed the double shuffle algebra $\mathfrak{dm}_0$ contained in $\mathfrak{mt}$ into a subspace of $\mathfrak{mq}$. To preserve the symmetries of these subspaces, we will need a more complicated embedding (cf Theorem 4.28).

3.3 Proof of the Key Lemma

To prove the Key Lemma 3.18, we need the following combinatorial identity.

Lemma 3.23. *Let $s \geq 1$, $m \geq 0$, $\theta_1, \dots, \theta_s \geq 0$ and $j \leq \theta_1 + \dots + \theta_s + m$, then we have*

$$\sum_{x_1=0}^{\theta_1} \cdots \sum_{x_s=0}^{\theta_s} \prod_{w=1}^{s} (-1)^{x_w} \binom{\theta_w}{x_w} \binom{m+\theta_1+\dots+\theta_s - x_1 - \dots - x_s}{j - x_1 - \dots - x_s} = \binom{m}{j}.$$

Proof. Observe that for $j < 0$ both sides of the equation are equal to 0, thus we can restrict to the case $j \geq 0$. To prove the equality consider the following generating series in $\mathbb{Q}[z_1, \dots, z_s]$

$$A(z_1,\dots,z_s) = \sum_{\theta_1,\dots,\theta_s \geq 0} a_{\theta_1,\dots,\theta_s} \frac{z_1^{\theta_1}}{\theta_1!} \cdots \frac{z_s^{\theta_s}}{\theta_s!}, \quad B(z_1,\dots,z_s) \ = \sum_{\theta_1,\dots,\theta_s \geq 0} b_{\theta_1,\dots,\theta_s} \frac{z_1^{\theta_1}}{\theta_1!} \cdots \frac{z_s^{\theta_s}}{\theta_s!}.$$

We compute directly that

$$\begin{aligned} &A(z_1,\dots,z_s)B(z_1,\dots,z_s) \\ &\qquad = \sum_{\theta_1,\dots,\theta_s \geq 0} \left(\sum_{x_1=0}^{\theta_1} \cdots \sum_{x_s=0}^{\theta_s} \binom{\theta_1}{x_1} \cdots \binom{\theta_s}{x_s} a_{x_1,\dots,x_s} b_{\theta_1 - x_1,\dots,\theta_s - x_s} \right) \frac{z_1^{\theta_1}}{\theta_1!} \cdots \frac{z_s^{\theta_s}}{\theta_s!}. \end{aligned}$$

For $\theta_1, \dots, \theta_s \geq 0$ and $j, m \geq 0$ set

$$a_{\theta_1,\dots,\theta_s} = \begin{cases} \frac{(-1)^{\theta_1+\dots+\theta_s}}{(j-\theta_1-\dots-\theta_s)!}, & j - \theta_1 - \dots - \theta_s \geq 0, \\ 0 & \text{else} \end{cases}, \qquad b_{\theta_1,\dots,\theta_s} = (m + \theta_1 + \dots + \theta_s)!.$$

Then we obtain from the previous formula

$$\begin{aligned} A(z_1,\dots,z_s)B(z_1,\dots,z_s) = \sum_{\theta_1,\dots,\theta_s \geq 0} \Bigg(&(m+\theta_1+\dots+\theta_s - j)! \sum_{x_1=0}^{\theta_1} \cdots \sum_{x_s=0}^{\theta_s} \binom{\theta_1}{x_1} \cdots \binom{\theta_s}{x_s} \\ &\cdot (-1)^{x_1+\dots+x_s} \binom{m+\theta_1+\dots+\theta_s - x_1 - \dots - x_s}{j - x_1 - \dots - x_s} \Bigg) \frac{z_1^{\theta_1}}{\theta_1!} \cdots \frac{z_s^{\theta_s}}{\theta_s!}. \end{aligned} \tag{3.23.1}$$

On the other hand, we deduce from the multinomial theorem

$$\begin{aligned} A(z_1,\dots,z_s) &= \frac{1}{j!} \sum_{\theta_1,\dots,\theta_s \geq 0} \binom{j}{\theta_1,\dots,\theta_s, j-\theta_1-\dots-\theta_s} (-z_1)^{\theta_1} \dots (-z_s)^{\theta_s} \\ &= \frac{1}{j!} (1 - z_1 - \dots - z_s)^j \end{aligned} \tag{3.23.2}$$

Next, we show that

$$B(z_1,\dots,z_s) = m! \sum_{\theta_1,\dots,\theta_s \geq 0} \binom{m+\theta_1+\dots+\theta_s}{m, \theta_1, \dots, \theta_s} z_1^{\theta_1} \dots z_s^{\theta_s} = m!(1 - z_1 - \dots - z_s)^{-(m+1)}. \tag{3.23.3}$$

The first equality follows from the definition of $B(z_1, \dots, z_s)$ and we prove the second equality by induction on m (where we omit the factor $m!$). If $m = 0$, then we obtain from the geometric series expansion and the multinomial theorem

$$\begin{aligned}(1-z_1-\cdots-z_s)^{-1} &= \sum_{k\geq 0}(z_1+\cdots+z_s)^k = \sum_{k\geq 0}\sum_{\theta_1+\cdots+\theta_s=k}\binom{k}{\theta_1,\ldots,\theta_s} z_1^{\theta_1}\ldots z_s^{\theta_s}\\ &= \sum_{\theta_1,\ldots,\theta_s\geq 0}\binom{\theta_1+\cdots+\theta_s}{\theta_1,\ldots,\theta_s} z_1^{\theta_1}\ldots z_s^{\theta_s}.\end{aligned}$$

Assume that (3.23.3) holds for some m. Then differentiating with respect to z_1 gives

$$\begin{aligned}(m+1)(1-z_1-\cdots-z_s)^{-(m+2)} &= \sum_{\theta_1\geq 1,\theta_2,\ldots,\theta_s\geq 0}\binom{m+\theta_1+\cdots+\theta_s}{m,\theta_1,\ldots,\theta_s}\theta_1 z_1^{\theta_1-1}z_2^{\theta_2}\ldots z_s^{\theta_s}\\ &= \sum_{\theta_1,\ldots,\theta_s\geq 0}\binom{m+1+\theta_1+\cdots+\theta_s}{m,\theta_1+1,\theta_2,\ldots,\theta_s}(\theta_1+1)z_1^{\theta_1}\ldots z_s^{\theta_s}\end{aligned}$$

and dividing by $(m+1)$ leads to

$$(1-z_1-\cdots-z_s)^{-(m+2)} = \sum_{\theta_1,\ldots,\theta_s\geq 0}\binom{m+1+\theta_1+\cdots+\theta_s}{m+1,\theta_1,\ldots,\theta_s} z_1^{\theta_1}\ldots z_s^{\theta_s}.$$

From (3.23.2) and (3.23.3) we deduce for $m \geq j$ that

$$\begin{aligned}A(z_1,\ldots,z_s)B(z_1,\ldots,z_s) &= \frac{m!}{j!}(1-z_1-\cdots-z_s)^{-(m+1-j)} \qquad (3.23.4)\\ &= \sum_{\theta_1,\ldots,\theta_s\geq 0}\frac{m!}{j!}\binom{m-j+\theta_1+\cdots+\theta_s}{m-j,\theta_1,\ldots,\theta_s} z_1^{\theta_1}\ldots z_s^{\theta_s}\\ &= \sum_{\theta_1,\ldots,\theta_s\geq 0}\binom{m}{j}(m-j+\theta_1+\cdots+\theta_s)!\frac{z_1^{\theta_1}}{\theta_1!}\cdots\frac{z_s^{\theta_s}}{\theta_s!}\end{aligned}$$

and for $m < j$ that

$$A(z_1,\ldots,z_s)B(z_1,\ldots,z_s) = \frac{m!}{j!}(1-z_1-\cdots-z_s)^{j-m-1}. \qquad (3.23.5)$$

Assume that $j \leq \theta_1+\cdots+\theta_s+m$, then coefficient comparison in (3.23.1) and (3.23.4), (3.23.5) gives

$$\begin{aligned}\sum_{x_1=0}^{\theta_1}\cdots\sum_{x_s=0}^{\theta_s}\prod_{w=1}^{s}(-1)^{x_w}\binom{\theta_w}{x_w}\binom{m+\theta_1+\cdots+\theta_s-x_1-\cdots-x_s}{j-x_1-\cdots-x_s} &= \begin{cases}\binom{m}{j}, & m\geq j,\\ 0, & m<j\end{cases}\\ &= \binom{m}{j}.\end{aligned}$$

For the first equality observe that the monomial $\frac{z_1^{\theta_1}}{\theta_1!}\cdots\frac{z_s^{\theta_s}}{\theta_s!}$ does not appear in (3.23.5) for $j-m\geq\theta_1+\cdots+\theta_s$. □

Now, we are able to give a proof of Key Lemma 3.18, this means we show

$$d^q_{\{f,g\}_q} = [d^q_f, d^q_g], \qquad f,g\in\mathbb{Q}\langle\mathcal{B}\rangle.$$

Proof. (of Key Lemma 3.18) Since we consider derivations on $\mathbb{Q}\langle\mathcal{B}\rangle$, the equality only needs to be shown on the generators b_i for $i \geq 0$. Evidently, we have for $f, g \in \mathbb{Q}\langle\mathcal{B}\rangle$

$$d^q_{\{f,g\}_q}(b_0) = 0 = [d^q_f, d^q_g](b_0).$$

Due to linearity, we can assume that $f = b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}$ and $g = b_0^{n_0} b_{l_1} b_0^{n_1} \dots b_{l_e} b_0^{n_e}$. Then we obtain for each $a \geq 1$ by the explicit formula in Lemma 3.13

$$\begin{aligned} d^q_{\{f,g\}_q}(b_a) = {} & A_1(f,g) + A_2(f,g) + A_3(f,g) + A_4(f,g) \\ & - A_1(g,f) - A_2(g,f) - A_3(g,f) - A_4(g,f) \\ & - A_5 - A_6, \end{aligned}$$

where (with the abbreviations $k = k_1 + \dots + k_d,\ l = l_1 + \dots + l_e,\ k' = k'_1 + \dots + k'_d,$ $s = s_1 + \dots + s_d,\ t = t_1 + \dots + t_e$)

$$\begin{aligned} A_1(f,g) = {} & \sum_{i=1}^{e} \sum_{k'_1=0}^{k_1-1} \cdots \sum_{k'_d=0}^{k_d-1} \sum_{s_1=0}^{k_1-k'_1-1} \cdots \sum_{s_d=0}^{k_d-k'_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_{i-1}=0}^{l_{i-1}-1} \sum_{t_i=0}^{l_i+k'-1} \sum_{t_{i+1}=0}^{l_{i+1}-1} \cdots \sum_{t_e=0}^{l_e-1} \\ & \cdot \prod_{u=1}^{d} (-1)^{k'_u+s_u} \binom{k_u-1}{k'_u} \binom{k_u-k'_u-1}{s_u} \prod_{\substack{v=1\\ v\neq i}}^{e} (-1)^{t_v} \binom{l_v-1}{t_v} (-1)^{t_i} \binom{l_i+k'-1}{t_i} \\ & \cdot \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_{i-1}-t_{i-1}} b_0^{n_{i-1}} \Big[b_0^{m_0} b_{k_1-k'_1-s_1} b_0^{m_1} \dots b_{k_d-k'_d-s_d} b_0^{m_d}, b_{l_i-t_i+k'} \Big] \\ & \qquad b_0^{n_i} b_{l_{i+1}-t_{i+1}} b_0^{n_{i+1}} \dots b_{l_e-t_e} b_0^{n_e}, b_{a+s+t} \Big], \end{aligned}$$

$$\begin{aligned} A_2(f,g) = {} & \sum_{i=1}^{e} \sum_{k'_1=0}^{k_1-1} \cdots \sum_{k'_d=0}^{k_d-1} \sum_{s_1=0}^{k_1-k'_1-1} \cdots \sum_{s_d=0}^{k_d-k'_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_{i-1}=0}^{l_{i-1}-1} \sum_{t_i=0}^{l_i+k'-1} \sum_{t_{i+1}=0}^{l_{i+1}-1} \cdots \sum_{t_e=0}^{l_e-1} \sum_{r=1}^{k+l-d-e} \sum_{h_1+\dots+h_{r+1}=s+t+1} \\ & \cdot (-1)^r \prod_{u=1}^{d} (-1)^{k'_u+s_u} \binom{k_u-1}{k'_u} \binom{k_u-k'_u-1}{s_u} \prod_{\substack{v=1\\ v\neq i}}^{e} (-1)^{t_v} \binom{l_v-1}{t_v} (-1)^{t_i} \binom{l_i+k'-1}{t_i} \\ & \cdot b_{a+h_1-1} b_{h_2} \dots b_{h_r} \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_{i-1}-t_{i-1}} b_0^{n_{i-1}} \Big[b_0^{m_0} b_{k_1-k'_1-s_1} b_0^{m_1} \dots b_{k_d-k'_d-s_d} b_0^{m_d}, b_{l_i-t_i+k'} \Big] \\ & \qquad b_0^{n_i} b_{l_{i+1}-t_{i+1}} b_0^{n_{i+1}} \dots b_{l_e-t_e} b_0^{n_e}, b_{h_{r+1}} \Big], \end{aligned}$$

$$\begin{aligned} A_3(f,g) = {} & \sum_{i=1}^{e} \sum_{k'_1=0}^{k_1-1} \cdots \sum_{k'_d=0}^{k_d-1} \sum_{s_1=0}^{k_1-k'_1-1} \cdots \sum_{s_d=0}^{k_d-k'_d-1} \sum_{p=1}^{k-d} \sum_{i_1+\dots+i_{p+1}=k'+1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_{i-1}=0}^{l_{i-1}-1} \sum_{t_i=0}^{l_i+i_1-2} \sum_{t_{i+1}=0}^{l_{i+1}-1} \cdots \sum_{t_e=0}^{l_e-1} \sum_{i'_2=0}^{i_2-1} \\ & \cdots \sum_{i'_{p+1}=0}^{i_{p+1}-1} (-1)^p \prod_{u=1}^{d} (-1)^{k'_u+s_u} \binom{k_u-1}{k'_u} \binom{k_u-k'_u-1}{s_u} \prod_{\substack{v=1\\ v\neq i}}^{e} (-1)^{t_v} \binom{l_v-1}{t_v} (-1)^{t_i} \binom{l_i+i_1-2}{t_i} \\ & \cdot \prod_{w=2}^{p+1} (-1)^{i'_w} \binom{i_w-1}{i'_w} \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_{i-1}-t_{i-1}} b_0^{n_{i-1}} b_{l_i-t_i+i_1-1} b_{i_2-i'_2} \dots b_{i_p-i'_p} \Big[b_0^{m_0} b_{k_1-k'_1-s_1} b_0^{m_1} \\ & \qquad \dots b_{k_d-k'_d-s_d} b_0^{m_d}, b_{i_{p+1}-i'_{p+1}} \Big] b_0^{n_i} b_{l_{i+1}-t_{i+1}} b_0^{n_{i+1}} \dots b_{l_e-t_e} b_0^{n_e}, b_{a+s+t+i'_2+\dots+i'_{p+1}} \Big], \end{aligned}$$

$$\begin{aligned}A_4(f,g)=&\sum_{i=1}^{e}\sum_{k_1'=0}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\sum_{s_1=0}^{k_1-k_1'-1}\cdots\sum_{s_d=0}^{k_d-k_d'-1}\sum_{p=1}^{k-d}\sum_{i_1+\cdots+i_{p+1}=k'+1}\sum_{t_1=0}^{l_1-1}\cdots\sum_{t_{i-1}=0}^{l_i-1}\sum_{t_i=0}^{l_i+i_1-2}\sum_{t_{i+1}=0}^{l_{i+1}-1}\cdots\sum_{t_e=0}^{l_e-1}\sum_{i_2'=0}^{i_2-1}\\&\cdots\sum_{i_{p+1}'=0}^{i_{p+1}-1}\sum_{r=1}^{k+l-d-e-p}\sum_{h_1+\cdots+h_{r+1}=s+t+i_2'+\cdots+i_{p+1}'+1}(-1)^{p+r}\prod_{u=1}^{d}(-1)^{k_u'+s_u}\binom{k_u-1}{k_u'}\binom{k_u-k_u'-1}{s_u}\\&\cdot\prod_{\substack{v=1\\v\neq i}}^{e}(-1)^{t_v}\binom{l_v-1}{t_v}(-1)^{t_i}\binom{l_i+i_1-2}{t_i}\prod_{w=2}^{p+1}(-1)^{i_w'}\binom{i_w-1}{i_w'}\\&\cdot b_{a+h_1-1}b_{h_2}\dots b_{h_r}\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_{i-1}-t_{i-1}}b_0^{n_{i-1}}b_{l_i-t_i+i_1-1}b_{i_2-i_2'}\dots b_{i_p-i_p'}\Big[b_0^{m_0}b_{k_1-k_1'-s_1}b_0^{m_1}\\&\qquad\dots b_{k_d-k_d'-s_d}b_0^{m_d},b_{i_{p+1}-i_{p+1}'}\Big]b_0^{n_i}b_{l_{i+1}-t_{i+1}}b_0^{n_{i+1}}\dots b_{l_e-t_e}b_0^{n_e},b_{h_{r+1}}\Big],\end{aligned}$$

and the $A_i(g,f)$ are obtained from the $A_i(f,g)$ by exchanging the roles of f and g (for $i=1,\dots,4$) and

$$\begin{aligned}A_5=&\sum_{k_1'=0}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\sum_{t_1=0}^{l_1-1}\cdots\sum_{t_e=0}^{l_e-1}\prod_{u=1}^{d}(-1)^{k_u'}\binom{k_u-1}{k_u'}\prod_{v=1}^{e}(-1)^{t_v}\binom{l_v-1}{t_v}\\&\cdot\Big[\Big[b_0^{m_0}b_{k_1-k_1'}b_0^{m_1}\dots b_{k_d-k_d'}b_0^{m_d},b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}\Big],b_{a+k'+t}\Big],\end{aligned}$$

$$\begin{aligned}A_6=&\sum_{k_1'=0}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\sum_{t_1=0}^{l_1-1}\cdots\sum_{t_e=0}^{l_e-1}\sum_{r=1}^{k+l-d-e}\sum_{h_1+\cdots+h_{r+1}=k'+t+1}(-1)^{r}\prod_{u=1}^{d}(-1)^{k_u'}\binom{k_u-1}{k_u'}\prod_{v=1}^{e}(-1)^{t_v}\binom{l_v-1}{t_v}\\&\cdot b_{a+h_1-1}b_{h_2}\dots b_{h_r}\Big[\Big[b_0^{m_0}b_{k_1-k_1'}b_0^{m_1}\dots b_{k_d-k_d'}b_0^{m_d},b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}\Big],b_{h_{r+1}}\Big].\end{aligned}$$

On the other hand, we obtain

$$\begin{aligned}d_f^q(d_g^q(b_a))-d_g^q(d_f^q(b_a))=&\,B_1(f,g)+B_2(f,g)+B_3(f,g)+B_4(f,g)\\&-B_1(g,f)-B_2(g,f)-B_3(g,f)-B_4(g,f)\\&+B_5+B_6,\end{aligned}$$

where (again with the abbreviations $k=k_1+\cdots+k_d,\ l=l_1+\cdots+l_e,\ k'=k_1'+\cdots+k_d'$, $s=s_1+\cdots+s_d,\ t=t_1+\cdots+t_e$)

$$\begin{aligned}B_1(f,g)=&\sum_{i=1}^{e}\sum_{k_1'=0}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\sum_{t_1=0}^{l_1-1}\cdots\sum_{t_e=0}^{l_e-1}\prod_{u=1}^{d}(-1)^{k_u'}\binom{k_u-1}{k_u'}\prod_{v=1}^{e}(-1)^{t_v}\binom{l_v-1}{t_v}\\&\cdot\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_{i-1}-t_{i-1}}b_0^{n_{i-1}}\Big[b_0^{m_0}b_{k_1-k_1'}b_0^{m_1}\dots b_{k_d-k_d'}b_0^{m_d},b_{l_i-t_i+k'}\Big]\\&\qquad b_0^{n_i}b_{l_{i+1}-t_{i+1}}b_0^{n_{i+1}}\dots b_{l_e-t_e}b_0^{n_e},b_{a+t}\Big],\end{aligned}$$

$$\begin{aligned}B_2(f,g)=&\sum_{i=1}^{e}\sum_{k_1'=0}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\sum_{t_1=0}^{l_1-1}\cdots\sum_{t_e=0}^{l_e-1}\sum_{p=1}^{l-e}\sum_{j_1+\cdots+j_{p+1}=t+1}(-1)^{p}\prod_{u=1}^{d}(-1)^{k_u'}\binom{k_u-1}{k_u'}\prod_{v=1}^{e}(-1)^{t_v}\binom{l_v-1}{t_v}\\&\cdot b_{a+j_1-1}b_{j_2}\dots b_{j_p}\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_{i-1}-t_{i-1}}b_0^{n_{i-1}}\Big[b_0^{m_0}b_{k_1-k_1'}b_0^{m_1}\dots b_{k_d-k_d'}b_0^{m_d},b_{l_i-t_i+k'}\Big]\\&\qquad b_0^{n_i}b_{l_{i+1}-t_{i+1}}b_0^{n_{i+1}}\dots b_{l_e-t_e}b_0^{n_e},b_{j_{p+1}}\Big],\end{aligned}$$

$$B_3(f,g) = \sum_{i=1}^{e} \sum_{k_1'=0}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_e=0}^{l_e-1} \sum_{p=1}^{k-d} \sum_{i_1+\cdots+i_{p+1}=k'+1} (-1)^p \prod_{u=1}^{d} (-1)^{k_u'} \binom{k_u-1}{k_u'} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v-1}{t_v}$$

$$\cdot \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_{i-1}-t_{i-1}} b_0^{n_{i-1}} b_{l_i-t_i+i_1-1} b_{i_2} \dots b_{i_p} \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, b_{i_{p+1}} \Big]$$

$$b_0^{n_i} b_{l_{i+1}-t_{i+1}} b_0^{n_{i+1}} \dots b_{l_e-t_e} b_0^{n_e}, b_{a+t} \Big],$$

$$B_4(f,g) = \sum_{i=1}^{e} \sum_{k_1'=0}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_e=0}^{l_e-1} \sum_{p_1=1}^{k-d} \sum_{i_1+\cdots+i_{p_1+1}=k'+1} \sum_{p_2=0}^{l-e} \sum_{j_1+\cdots+j_{p_2+1}=t+1} (-1)^{p_1+p_2}$$

$$\cdot \prod_{u=1}^{d} (-1)^{k_u'} \binom{k_u-1}{k_u'} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v-1}{t_v} b_{a+j_1-1} b_{j_2} \dots b_{j_{p_2}} \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_{i-1}-t_{i-1}} b_0^{n_{i-1}}$$

$$b_{l_i-t_i+i_1-1} b_{i_2} \dots b_{i_{p_1}} \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, b_{i_{p_1+1}} \Big] b_0^{n_i} b_{l_{i+1}-t_{i+1}} b_0^{n_{i+1}} \dots b_{l_e-t_e} b_0^{n_e}, b_{j_{p_2+1}} \Big],$$

the terms $B_i(g,f)$ are obtained from $B_i(f,g)$ by exchanging the roles of f and g ($i = 1, \dots 4$), and

$$B_5 = \sum_{k_1'=0}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_e=0}^{l_e-1} \prod_{u=1}^{d} (-1)^{k_u'} \binom{k_u-1}{k_u'} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v-1}{t_v}$$

$$\cdot \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_e-t_e} b_0^{n_e}, \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, b_{a+k'+t} \Big] \Big]$$

$$- \sum_{k_1'=0}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_e=0}^{l_e-1} \prod_{u=1}^{d} (-1)^{k_u'} \binom{k_u-1}{k_u'} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v-1}{t_v}$$

$$\cdot \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_e-t_e} b_0^{n_e}, b_{a+k'+t} \Big] \Big]$$

$$B_6 = \sum_{k_1'=0}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_e=0}^{l_e-1} \sum_{p=1}^{k-d} \sum_{i_1+\cdots+i_{p+1}=k'+1} (-1)^p \prod_{u=1}^{d} (-1)^{k_u'} \binom{k_u-1}{k_u'} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v-1}{t_v}$$

$$\cdot \Bigg(b_{a+t+i_1-1} \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_e-t_e} b_0^{n_e}, b_{i_2} \dots b_{i_p} \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, b_{i_{p+1}} \Big] \Big]$$

$$- \sum_{x=2}^{p} b_{a+i_1-1} b_{i_2} \dots b_{i_{x-1}} \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_e-t_e} b_0^{n_e}, b_{i_x+t} \Big] b_{i_{x+1}} \dots b_{i_p} \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, b_{i_{p+1}} \Big]$$

$$- b_{a+i_1-1} b_{i_2} \dots b_{i_p} \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_e-t_e} b_0^{n_e}, b_{i_{p+1}+t} \Big] \Big] \Bigg)$$

$$+ \sum_{k_1'=0}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_e=0}^{l_e-1} \sum_{p=1}^{l-e} \sum_{j_1+\cdots+j_{p+1}=t+1} (-1)^p \prod_{u=1}^{d} (-1)^{k_u'} \binom{k_u-1}{k_u'} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v-1}{t_v}$$

$$\cdot \Bigg(- b_{a+k'+j_1-1} \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, b_{j_2} \dots b_{j_p} \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_e-t_e} b_0^{n_e}, b_{j_{p+1}} \Big] \Big]$$

$$+ \sum_{x=2}^{p} b_{a+j_1-1} b_{j_2} \dots b_{j_{x-1}} \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, b_{j_x+k'} \Big] b_{j_{x+1}} \dots b_{j_p} \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_e-t_e} b_0^{n_e}, b_{j_{p+1}} \Big]$$

$$+ b_{a+j_1-1} b_{j_2} \dots b_{j_p} \Big[b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \dots b_{l_e-t_e} b_0^{n_e}, \Big[b_0^{m_0} b_{k_1-k_1'} b_0^{m_1} \dots b_{k_d-k_d'} b_0^{m_d}, b_{j_{p+1}+k'} \Big] \Big] \Bigg)$$

$$+ \sum_{k_1'=0}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \sum_{t_1=0}^{l_1-1} \cdots \sum_{t_e=0}^{l_e-1} \sum_{p_1=1}^{k-d} \sum_{i_1+\cdots+i_{p_1+1}=k'+1} \sum_{p_2=1}^{l-e} \sum_{j_1+\cdots+j_{p_2+1}=t+1} (-1)^{p_1+p_2}$$

$$\cdot \prod_{u=1}^{d}(-1)^{k'_u}\binom{k_u-1}{k'_u}\prod_{v=1}^{e}(-1)^{t_v}\binom{l_v-1}{t_v}$$

$$\cdot \Bigg(b_{a+i_1+j_1-2}b_{i_2}\dots b_{i_{p_1}}\Big[b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}, b_{i_{p_1+1}}\Big]b_{j_2}\dots b_{j_{p_2}}\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}, b_{j_{p_2+1}}\Big]$$

$$-\sum_{x=2}^{p_1} b_{a+i_1-1}b_{i_2}\dots b_{i_{x-1}}b_{i_x+j_1-1}b_{j_2}\dots b_{j_{p_2}}\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}, b_{j_{p_2+1}}\Big]b_{i_{x+1}}\dots b_{i_{p_1}}$$

$$\Big[b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}, b_{i_{p_1+1}}\Big]$$

$$-\, b_{a+i_1-1}b_{i_2}\dots b_{i_{p_1}}\Big[b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}, b_{i_{p_1+1}+j_1-1}b_{j_2}\dots b_{j_{p_2}}\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}, b_{j_{p_2+1}}\Big]\Big]$$

$$-\, b_{a+i_1+j_1-2}b_{j_2}\dots b_{j_{p_2}}\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}, b_{j_{p_2+1}}\Big]b_{i_2}\dots b_{i_{p_1}}\Big[b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}, b_{i_{p_1+1}}\Big]$$

$$+\sum_{x=2}^{p_2} b_{a+j_1-1}b_{j_2}\dots b_{j_{x-1}}b_{j_x+i_1-1}b_{i_2}\dots b_{i_{p_1}}\Big[b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}, b_{i_{p_1+1}}\Big]b_{j_{x+1}}\dots b_{j_{p_2}}$$

$$\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}, b_{j_{p_2+1}}\Big]$$

$$+\, b_{a+j_1-1}b_{j_2}\dots b_{j_{p_2}}\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}, b_{j_{p_2+1}+i_1-1}b_{i_2}\dots b_{i_{p_1}}\Big[b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}, b_{i_{p_1+1}}\Big]\Big]\Bigg).$$

We will show successively that $A_i(f,g) = B_i(f,g)$ for $i = 1,\dots,4$, and $-A_i = B_i$ for $i = 5,6$.

We start by showing the equality $A_1(f,g) = B_1(f,g)$. For $i \in \{1,\dots,e\}$, $t_v \in \{0,\dots,l_v-1\}$ for $v = 1,\dots,i-1,i+1,\dots,e$, $\sigma_u \in \{0,\dots,k_u-1\}$ for $u = 1,\dots,d$ and $\tau \in \{-(k-d),\dots,l_i-1\}$, the coefficient of

$$\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_{i-1}-t_{i-1}}b_0^{n_{i-1}}\Big[b_0^{m_0}b_{k_1-\sigma_1}b_0^{m_1}\dots b_{k_d-\sigma_d}b_0^{m_d}, b_{l_i-\tau}\Big]b_0^{n_i}b_{l_{i+1}-t_{i+1}}b_0^{n_{i+1}}$$

$$\dots b_{l_e-t_e}b_0^{n_e}, b_{a+t_1+\dots+t_{i-1}+t_{i+1}+\dots+t_e+\tau+\sigma_1+\dots+\sigma_d}\Big]$$

in $A_1(f,g)$ is given by

$$(-1)^{t_1+\dots+t_{i-1}+t_{i+1}+\dots+t_e+\tau}\sum_{x_1=0}^{\sigma_1}\dots\sum_{x_d=0}^{\sigma_d}\prod_{u=1}^{d}(-1)^{x_u+\sigma_u}\binom{k_u-1}{x_u}\binom{k_u-x_u-1}{\sigma_u-x_u}$$

$$\cdot\binom{l_i+x_1+\dots+x_d-1}{\tau+x_1+\dots+x_d}\prod_{\substack{v=1\\v\neq i}}^{e}\binom{l_v-1}{t_v}$$

and the coefficient in $B_1(f,g)$ is given by

$$(-1)^{t_1+\dots+t_{i-1}+t_{i+1}+\dots+t_e+\tau}\prod_{u=1}^{d}\binom{k_u-1}{\sigma_u}\binom{l_i-1}{\tau+\sigma_1+\dots+\sigma_d}\prod_{\substack{v=1\\v\neq i}}^{e}\binom{l_v-1}{t_v}.$$

Therefore, we have to show that

$$\sum_{x_1=0}^{\sigma_1}\dots\sum_{x_d=0}^{\sigma_d}\prod_{u=1}^{d}(-1)^{x_u+\sigma_u}\binom{k_u-1}{x_u}\binom{k_u-x_u-1}{\sigma_u-x_u}\binom{l_i+x_1+\dots+x_d-1}{\tau+x_1+\dots+x_d}$$

$$=\prod_{u=1}^{d}\binom{k_u-1}{\sigma_u}\binom{l_i-1}{\tau+\sigma_1+\dots+\sigma_d}.$$

Applying the identity $\binom{k_u-1}{x_u}\binom{k_u-x_u-1}{\sigma_u-x_u} = \binom{k_u-1}{\sigma_u}\binom{\sigma_u}{x_u}$ and substituting $x_u \mapsto \sigma_u - x_u$ simplifies the equality to

$$\sum_{x_1=0}^{\sigma_1}\cdots\sum_{x_d=0}^{\sigma_d}\prod_{u=1}^{d}(-1)^{x_u}\binom{\sigma_u}{x_u}\binom{l_i-1+\sigma_1+\cdots+\sigma_d-x_1-\cdots-x_d}{\tau+\sigma_1+\cdots+\sigma_d-x_1-\cdots-x_d}$$
$$=\binom{l_i-1}{\tau+\sigma_1+\cdots+\sigma_d}.$$

This equation follows from Lemma 3.23 substituting $s=d$, $m=l_i-1$, $\theta_u=\sigma_u$ for $u=1,\ldots,d$ and $j=\tau+\sigma_1+\cdots+\sigma_d$.

Next, we show that $A_2(f,g)=B_2(f,g)$. For $i\in\{1,\ldots,e\}$, $t_v\in\{0,\ldots l_v-1\}$ for $v=1,\ldots,i-1,i+1,\ldots,e$, $\sigma_u\in\{0,\ldots,k_u-1\}$ for $u=1,\ldots,d$, $\tau\in\{-(k-d),\ldots,l_i-1\}$, $r\in\{1,\ldots,k+l-d-e\}$ and $h_1+\cdots+h_{r+1}=t_1+\cdots+t_{i-1}+t_{i+1}+\cdots+t_e+\sigma_1+\cdots+\sigma_d+\tau$, the coefficient of

$$b_{a+h_1-1}b_{h_2}\ldots b_{h_r}\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\ldots b_{l_{i-1}-t_{i-1}}b_0^{n_{i-1}}\Big[b_0^{m_0}b_{k_1-\sigma_1}b_0^{m_1}\ldots b_{k_d-\sigma_d}b_0^{m_d},b_{l_i-\tau}\Big]$$
$$\cdot\, b_0^{n_i}b_{l_{i+1}-t_{i+1}}b_0^{n_{i+1}}\ldots b_{l_e-t_e}b_0^{n_e},b_{h_{r+1}}\Big]$$

in $A_2(f,g)$ is given by

$$(-1)^{t_1+\cdots+t_{i-1}+t_{i+1}+\cdots+t_e+\tau+r}\sum_{x_1=0}^{\sigma_1}\cdots\sum_{x_d=0}^{\sigma_d}\prod_{u=1}^{d}(-1)^{x_u+\sigma_u}\binom{k_u-1}{x_u}\binom{k_u-x_u-1}{\sigma_u-x_u}$$
$$\cdot\binom{l_i+x_1+\cdots+x_d-1}{\tau+x_1+\cdots+x_d}\prod_{\substack{v=1\\v\neq i}}^{e}\binom{l_v-1}{t_v}$$

and the coefficient in $B_2(f,g)$ is

$$(-1)^{t_1+\cdots+t_{i-1}+t_{i+1}+\cdots+t_e+\tau+r}\prod_{u=1}^{d}\binom{k_u-1}{\sigma_u}\binom{l_i-1}{\tau+\sigma_1+\cdots+\sigma_d}\prod_{\substack{v=1\\v\neq i}}^{e}\binom{l_v-1}{t_v}.$$

In particular, the equality $A_2(f,g)=B_2(f,g)$ is proven similar to the previous case $A_1(f,g)=B_1(f,g)$.

We want to show that $A_3(f,g)=B_3(f,g)$. For $i\in\{1,\ldots,e\}$, $t_v\in\{0,\ldots l_v-1\}$ for $v=1,\ldots,i-1,i+1,\ldots,e$, $\sigma_u\in\{0,\ldots,k_u-1\}$ for $u=1,\ldots,d$, $r\in\{1,\ldots,k-d\}$ and $\iota+\iota_2+\cdots+\iota_{r+1}\leq\sigma_1+\cdots+\sigma_d+l_i-1$, the coefficient of

$$\Big[b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\ldots b_{l_{i-1}-t_{i-1}}b_0^{n_{i-1}}b_{l_i-\iota-1}b_{\iota_2}\ldots b_{\iota_r}\Big[b_0^{m_0}b_{k_1-\sigma_1}b_0^{m_1}\ldots b_{k_d-\sigma_d}b_0^{m_d},b_{\iota_{r+1}}\Big]$$
$$\cdot\, b_0^{n_i}b_{l_{i+1}-t_{i+1}}b_0^{n_{i+1}}\ldots b_{l_e-t_e}b_0^{n_e},b_{a+t_1+\cdots+t_{i-1}+t_{i+1}+\cdots+t_e+\sigma_1+\cdots+\sigma_d+\iota-\iota_2-\cdots-\iota_{r+1}+1}\Big]$$

in $A_3(f,g)$ is

$$(-1)^{t_1+\cdots+t_{i-1}+t_{i+1}+\cdots+t_e+\iota-\iota_2-\cdots-\iota_{r+1}+r+1}\sum_{x_1=0}^{\sigma_1}\cdots\sum_{x_d=0}^{\sigma_d}\sum_{\substack{y_1+\cdots+y_{r+1}=x_1+\cdots+x_d+1\\y_j\geq1}}\prod_{u=1}^{d}(-1)^{x_u+\sigma_u}$$
$$\cdot\binom{k_u-1}{x_u}\binom{k_u-x_u-1}{\sigma_u-x_u}\binom{l_i+y_1-2}{y_1+\iota}\binom{y_2-1}{y_2-\iota_2}\cdots\binom{y_{r+1}-1}{y_{r+1}-\iota_{r+1}}\prod_{\substack{v=1\\v\neq i}}^{e}\binom{l_v-1}{t_v}$$

and the coefficient in $B_3(f,g)$ is

$$(-1)^{t_1+\cdots+t_{i-1}+t_{i+1}+\cdots+t_e+\iota-\iota_2-\cdots-\iota_{r+1}+r+1}\prod_{u=1}^{d}\binom{k_u-1}{\sigma_u} \cdot\binom{l_i-1}{\sigma_1+\cdots+\sigma_d+1+\iota-\iota_2-\cdots-\iota_{r+1}}\prod_{\substack{v=1\\v\neq i}}^{e}\binom{l_v-1}{t_v}$$

Therefore, we have to show that

$$\sum_{x_1=0}^{\sigma_1}\cdots\sum_{x_d=0}^{\sigma_d}\sum_{\substack{y_1+\cdots+y_{r+1}=x_1+\cdots+x_d+1\\y_j\geq 1}}\prod_{u=1}^{d}(-1)^{x_u+\sigma_u}\binom{\sigma_u}{x_u}\binom{l_i+y_1-2}{y_1+\iota} \cdot\binom{y_2-1}{y_2-\iota_2}\cdots\binom{y_{r+1}-1}{y_{r+1}-\iota_{r+1}}=\binom{l_i-1}{\sigma_1+\cdots+\sigma_d+1+\iota-\iota_2-\cdots-\iota_{r+1}}.$$

Substituting $s=d$, $m=l_i-1$, $\theta_u=\sigma_u$ for $u=1,\ldots,d$ and $j=\sigma_1+\cdots+\sigma_d+1+\iota-\iota_2-\cdots-\iota_{r+1}$ in Lemma 3.23 yields

$$\begin{aligned}&\binom{l_i-1}{\sigma_1+\cdots+\sigma_d+1+\iota-\iota_2-\cdots-\iota_{r+1}}\\&=\sum_{x_1=0}^{\sigma_1}\cdots\sum_{x_d=0}^{\sigma_d}\prod_{u=1}^{d}(-1)^{x_u}\binom{\sigma_u}{x_u}\binom{l_i-1+\sigma_1+\cdots+\sigma_d-x_1-\cdots-x_d}{\sigma_1+\cdots+\sigma_d+1+\iota-\iota_2-\cdots-\iota_{r+1}-x_1-\cdots-x_d}\\&=\sum_{x_1=0}^{\sigma_1}\cdots\sum_{x_d=0}^{\sigma_d}\prod_{u=1}^{d}(-1)^{x_u+\sigma_u}\binom{\sigma_u}{x_u}\binom{l_i-1+x_1+\cdots+x_d}{\iota-\iota_2-\cdots-\iota_{r+1}+1+x_1+\cdots+x_d}.\end{aligned}$$

Thus, we are left with showing that we have with $x=x_1+\cdots+x_d$

$$\sum_{\substack{y_1+\cdots+y_{r+1}=x+1\\y_j\geq 1}}\binom{l_i+y_1-2}{y_1+\iota}\binom{y_2-1}{y_2-\iota_2}\cdots\binom{y_{r+1}-1}{y_{r+1}-\iota_{r+1}}=\binom{l_i-1+x}{\iota-\iota_2-\cdots-\iota_{r+1}+1+x}.$$

To prove this equality consider the following generating series

$$\begin{aligned}\sum_{y\geq 0}\binom{y+l_i-2-\iota+\iota_2+\cdots+\iota_{r+1}}{l_i-2-\iota+\iota_2+\cdots+\iota_{r+1}}z^y&=(1-z)^{-(l_i-1-\iota+\iota_2+\cdots+\iota_{r+1})}\\&=(1-z)^{-(l_i-1-\iota)}(1-z)^{-\iota_2}\ldots(1-z)^{-\iota_{r+1}}\\&=\sum_{y_1,\ldots,y_{r+1}\geq 0}\binom{y_1+l_i-2-\iota}{l_i-2-\iota}\binom{y_2+\iota_2-1}{\iota_2-1}\cdots\binom{y_{r+1}+\iota_{r+1}-1}{\iota_{r+1}-1}z^{y_1}\ldots z^{y_{r+1}},\end{aligned}\tag{3.23.6}$$

where we made use of the identity $\sum_{y\geq 0}\binom{m+y}{m}z^y=(1-z)^{-(m+1)}$ (cf (3.23.3)). Coefficient comparison in (3.23.6) at $z^{x+\iota-\iota_2-\cdots-\iota_{r+1}+1}$ yields

$$\begin{aligned}&\binom{l_i-1+x}{l_i-2-\iota+\iota_2+\cdots+\iota_{r+1}}\\&=\sum_{\substack{y_1+\cdots+y_{r+1}=x+\iota-\iota_2-\cdots-\iota_{r+1}+1\\y_j\geq 0}}\binom{y_1+l_i-2-\iota}{l_i-2-\iota}\binom{y_2+\iota_2-1}{\iota_2-1}\cdots\binom{y_{r+1}+\iota_{r+1}-1}{\iota_{r+1}-1},\end{aligned}$$

which simplifies to (substitute $y_1 \mapsto y_1 + \iota$, $y_j \mapsto y_j - \iota_j$ for $j = 2, \dots, r+1$)

$$\binom{l_i - 1 + x}{\iota - \iota_2 - \cdots - \iota_{r+1} + 1 + x} = \sum_{\substack{y_1 + \cdots + y_{r+1} = x+1 \\ y_j \geq 1}} \binom{l_i + y_1 - 2}{y_1 + \iota} \binom{y_2 - 1}{y_2 - \iota_2} \cdots \binom{y_{r+1} - 1}{y_{r+1} - \iota_{r+1}}.$$

This proves $A_3(f, g) = B_3(f, g)$. Again the equation $A_4(f, g) = B_4(f, g)$ follows similarly to this case.

Applying Jacobi's identity for the commutator bracket, one easily obtains $A_5 + B_5 = 0$ and hence the desired equality $-A_5 = B_5$.

Finally, we will show that $-A_6 = B_6$. Any word occurring in A_6 or B_6 is of the form

$$b_{a+x_1} b_{x_2} \dots b_{x_{w_1}} b_0^{m_0} b_{k_1 - k_1'} b_0^{m_1} \dots b_{k_d - k_d'} b_0^{m_d} b_{y_1} \dots b_{y_{w_2}} b_0^{n_0} b_{l_1 - t_1} b_0^{n_1} \dots b_{l_e - t_e} b_0^{n_e} b_{z_1} \dots b_{z_{w_3}} \tag{3.23.7}$$

or

$$b_{a+x_1} b_{x_2} \dots b_{x_{w_1}} b_0^{n_0} b_{l_1 - t_1} b_0^{n_1} \dots b_{l_e - t_e} b_0^{n_e} b_{y_1} \dots b_{y_{w_2}} b_0^{m_0} b_{k_1 - k_1'} b_0^{m_1} \dots b_{k_d - k_d'} b_0^{m_d} b_{z_1} \dots b_{z_{w_3}}$$

for some $k_u' \in \{0, \dots, k_u - 1\}$ for $u = 1, \dots, d$, $t_v \in \{0, \dots, l_v - 1\}$ for $v = 1, \dots, e$, $w_1 \geq 1$, $w_2 \geq 0$, $w_3 \in \{0, 1\}$ and $x_1 + \cdots + x_{w_1} + y_1 + \cdots + y_{w_2} + z_1 + \cdots + z_{w_3} = k' + t$. We will focus on the first case (3.23.7), the second case is proven completely similar due to anti-symmetry. If $w_2 = w_3 = 0$, the part of $-A_6$ containing words of the form (3.23.7) is given by

$$(-1)^{w_1 - 1} \prod_{u=1}^{d} (-1)^{k_u'} \binom{k_u - 1}{k_u'} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v - 1}{t_v} \sum_{h_1 + \cdots + h_{w_1} = k' + t + 1} \cdot b_{a+h_1-1} b_{h_2} \dots b_{h_{w_1}} b_0^{m_0} b_{k_1 - k_1'} b_0^{m_1} \dots b_{k_d - k_d'} b_0^{m_d} b_0^{n_0} b_{l_1 - t_1} b_0^{n_1} \dots b_{l_e - t_e} b_0^{n_e} \tag{3.23.8}$$

and the part of B_6 containing words of the form (3.23.7) is

$$\begin{aligned} &(-1)^{w_1 - 1} \prod_{u=1}^{d} (-1)^{k_u'} \binom{k_u - 1}{k_u'} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v - 1}{t_v} \\ &\cdot \Bigg(\sum_{i_1 + \cdots + i_{w_1} = k' + 1} b_{a+t+i_1-1} b_{i_2} \cdots {}_{i_{w_1}} b_0^{m_0} b_{k_1 - k_1'} b_0^{m_1} \dots b_{k_d - k_d'} b_0^{m_d} b_0^{n_0} b_{l_1 - t_1} b_0^{n_1} \dots b_{l_e - t_e} b_0^{n_e} \\ &+ \sum_{j_1 + \cdots + j_{w_1} = t+1} b_{a+j_1-1} b_{j_2} \dots b_{j_{w_1}} b_0^{m_0} b_{k_1 - k_1'} b_0^{m_1} \dots b_{k_d - k_d'} b_0^{m_d} b_0^{n_0} b_{l_1 - t_1} b_0^{n_1} \dots b_{l_e - t_e} b_0^{n_e} \\ &+ \sum_{w_1' = 2}^{w_1 - 1} \sum_{i_1 + \cdots + i_{w_1 - w_1' + 1} = k' + 1} \sum_{j_1 + \cdots + j_{w_1'} = t+1} b_{a+j_1-1} b_{j_2} \dots b_{j_{w_1' - 1}} b_{j_{w_1'} + i_1 - 1} b_{i_2} \dots b_{i_{w_1 - w_1' + 1}} \\ &\qquad \cdot b_0^{m_0} b_{k_1 - k_1'} b_0^{m_1} \dots b_{k_d - k_d'} b_0^{m_d} b_0^{n_0} b_{l_1 - t_1} b_0^{n_1} \dots b_{l_e - t_e} b_0^{n_e} \Bigg). \end{aligned} \tag{3.23.9}$$

The three terms together in (3.23.9) give exactly all possibilities for the decomposition in (3.23.8), thus these two terms agree.
Next we consider the case $w_2 = 1$, $w_3 = 0$, then in $-A_6$ occur no words of the form (3.23.7) and the part of B_6 containing words of the form (3.23.7) is given by

$$(-1)^{w_1}\prod_{u=1}^{d}(-1)^{k'_u}\binom{k_u-1}{k'_u}\prod_{v=1}^{e}(-1)^{t_v}\binom{l_v-1}{t_v}$$

$$\cdot\Bigg(-\sum_{i_1+\cdots+i_{w_1}+i=k'+1} b_{a+t+i_1-1}b_{i_2}\dots b_{i_{w_1}}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_ib_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$+\sum_{i_1+\cdots+i_{w_1}+i=k'+1} b_{a+i_1-1}b_{i_2}\dots b_{i_{w_1}}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_{i+t}b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$+\sum_{j_1+\cdots+j_{w_1}+j=t+1} b_{a+j_1-1}b_{j_2}\dots b_{j_{w_1-1}}b_{j_{w_1}+k'}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_jb_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$-\sum_{j_1+\cdots+j_{w_1}+j=t+1} b_{a+j_1-1}b_{j_2}\dots b_{j_{w_1}}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_{j+k'}b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$+\sum_{i_1+\cdots+i_{w_1}=k'+1}\ \sum_{j_1+j=t+1} b_{a+i_1+j_1-1}b_{i_2}\dots b_{i_{w_1}}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_jb_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$+\sum_{w'_1=2}^{w_1-1}\ \sum_{i_1+\cdots+i_{w_1-w'_1+1}=k'+1}\ \sum_{j_1+\cdots+j_{w'_1}+j=t+1} b_{a+j_1-1}b_{j_2}\dots b_{j_{w'_1-1}}b_{j_{w'_1}+i_1-1}b_{i_2}\dots b_{i_{w_1-w'_1+1}}$$

$$\cdot b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_jb_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$-\sum_{w'_1=2}^{w_1}\ \sum_{i_1+\cdots+i_{w_1-w'_1+1}+i=k'+1}\ \sum_{j_1+\cdots+j_{w'_1}=t+1} b_{a+j_1-1}b_{j_2}\dots b_{j_{w'_1-1}}b_{j_{w'_1}+i_1-1}b_{i_2}\dots b_{i_{w_1-w'_1+1}}$$

$$\cdot b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_ib_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}\Bigg)$$

As in the previous case, the sum of the second, third, fifth, and sixth terms is equal to

$$\sum_{h_1+\cdots+h_{w_1}+h=k'+t+1} b_{a+h_1-1}b_{h_2}\dots b_{h_{w_1}}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_hb_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e} \tag{3.23.10}$$

and the sum of the first, fourth, and seventh terms is equal to the negative of (3.23.10). Thus the terms in B_6, which are of the form (3.23.7) with $w_2=1,\ w_3=0$ cancel out.
Next, we consider the case $w_1=1,\ w_2\geq 2,\ w_3=0$. Again there are no words in $-A_6$, which are of the form (3.23.7). Moreover, the parts in B_6 having the form in (3.23.7) are

$$(-1)^{w_2}\prod_{u=1}^{d}(-1)^{k'_u}\binom{k_u-1}{k'_u}\prod_{v=1}^{e}(-1)^{t_v}\binom{l_v-1}{t_v}$$

$$\cdot\Bigg(\sum_{j+j_1+\cdots+j_{w_2}=t+1} b_{a+k'+j-1}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_{j_1}\dots b_{j_{w_2}}b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$-\sum_{j+j_1+\cdots+j_{w_2}=t+1} b_{a+j-1}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_{j_1+k'}b_{j_2}\dots b_{j_{w_2}}b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$-\sum_{i_1+i_2=k'+1}\ \sum_{j+j_1+\cdots+j_{w_2-1}=t+1} b_{a+i_1+j-2}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}$$

$$\cdot b_{i_2}b_{j_1}\dots b_{j_{w_2-1}}b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}$$

$$+\sum_{i_1+i_2=k'+1}\ \sum_{j_1+\cdots+j_{w_2}=t+1} b_{a+i_1-1}b_0^{m_0}b_{k_1-k'_1}b_0^{m_1}\dots b_{k_d-k'_d}b_0^{m_d}b_{i_2+j_1-1}$$

$$\cdot b_{j_2}\dots b_{j_{w_2}}b_0^{n_0}b_{l_1-t_1}b_0^{n_1}\dots b_{l_e-t_e}b_0^{n_e}\Bigg).$$

As before, the sum of the first and fourth terms and the sum of the second and third terms cancel out, therefore also B_6 has no terms of the form (3.23.7) (if $w_1 = 1,\ w_2 \geq 2$, and $w_3 = 0$).
Finally, we consider the case $w_1, w_2 \geq 2,\ w_3 = 0$. Then there are no words in $-A_6$, which are of the form (3.23.7), and the parts in B_6 of the form (3.23.7) are given by

$$
\begin{aligned}
&(-1)^{w_2} \prod_{u=1}^{d} (-1)^{k'_u} \binom{k_u - 1}{k'_u} \prod_{v=1}^{e} (-1)^{t_v} \binom{l_v - 1}{t_v} \\
&\quad \cdot \Bigg(- \sum_{j_1+\cdots+j_{w_1+w_2}=t+1} b_{a+j_1-1} b_{j_2} \ldots b_{j_{w_1}} b_0^{m_0} b_{k_1-k'_1} b_0^{m_1} \ldots b_{k_d-k'_d} b_0^{m_d} b_{j_{w_1+1}+k'} b_{j_{w_1+2}} \\
&\qquad\qquad \ldots b_{j_{w_1+w_2}} b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \ldots b_{l_e-t_e} b_0^{n_e} \\
&+ \sum_{j_1+\cdots+j_{w_1+w_2}=t+1} b_{a+j_1-1} b_{j_2} \ldots b_{j_{w_1-1}} b_{j_{w_1}+k'} b_0^{m_0} b_{k_1-k'_1} b_0^{m_1} \ldots b_{k_d-k'_d} b_0^{m_d} b_{j_{w_1+1}} \ldots b_{j_{w_1+w_2}} \\
&\qquad\qquad \cdot b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \ldots b_{l_e-t_e} b_0^{n_e} \\
&- \sum_{i_1+\cdots+i_{w_1}+i=k'+1} \ \sum_{j+j_1+\cdots+j_{w_2-1}=t+1} b_{a+i_1+j-2} b_{i_2} \ldots b_{i_{w_1}} b_0^{m_0} b_{k_1-k'_1} b_0^{m_1} \ldots b_{k_d-k'_d} b_0^{m_d} b_i b_{j_1} \\
&\qquad\qquad \ldots b_{j_{w_2-1}} b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \ldots b_{l_e-t_e} b_0^{n_e} \\
&+ \sum_{i_1+\cdots+i_{w_1}=k'+1} \ \sum_{j+j_1+\cdots+j_{w_2}=t+1} b_{a+i_1+j-2} b_{i_2} \ldots b_{i_{w_1}} b_0^{m_0} b_{k_1-k'_1} b_0^{m_1} \ldots b_{k_d-k'_d} b_0^{m_d} b_{j_1} \\
&\qquad\qquad \ldots b_{j_{w_2}} b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \ldots b_{l_e-t_e} b_0^{n_e} \\
&+ \sum_{i_1+\cdots+i_{w_1}+i=k'+1} \ \sum_{j_1+\cdots+j_{w_2}=t+1} b_{a+i_1-1} b_{i_2} \ldots b_{i_{w_1}} b_0^{m_0} b_{k_1-k'_1} b_0^{m_1} \ldots b_{k_d-k'_d} b_0^{m_d} b_{i+j_1-1} b_{j_2} \\
&\qquad\qquad \ldots b_{j_{w_2}} b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \ldots b_{l_e-t_e} b_0^{n_e} \\
&- \sum_{w'_1=1}^{w_1-1} \ \sum_{i_1+\cdots+i_{w'_1}+i=k'+1} \ \sum_{j_1+\cdots+j_{w_1-w'_1+w_2}=t+1} b_{a+j_1-1} b_{j_2} \ldots b_{j_{w_1-w'_1}} b_{j_{w_1-w'_1+1}+i_1-1} b_{i_2} \\
&\qquad \ldots b_{i_{w'_1}} b_0^{m_0} b_{k_1-k'_1} b_0^{m_1} \ldots b_{k_d-k'_d} b_0^{m_d} b_i b_{j_{w_1-w'_1+2}} \ldots b_{j_{w_1-w'_1+w_2}} b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \ldots b_{l_e-t_e} b_0^{n_e} \\
&+ \sum_{w'_1=2}^{w_1-1} \ \sum_{i_1+\cdots+i_{w'_1}=k'+1} \ \sum_{j_1+\cdots+j_{w_1-w'_1+w_2+1}=t+1} b_{a+j_1-1} b_{j_2} \ldots b_{j_{w_1-w'_1}} b_{j_{w_1-w'_1+1}+i_1-1} b_{i_2} \\
&\qquad \ldots b_{i_{w'_1}} b_0^{m_0} b_{k_1-k'_1} b_0^{m_1} \ldots b_{k_d-k'_d} b_0^{m_d} b_{j_{w_1-w'_1+2}} \ldots b_{j_{w_1-w'_1+w_2+1}} b_0^{n_0} b_{l_1-t_1} b_0^{n_1} \ldots b_{l_e-t_e} b_0^{n_e} \Bigg).
\end{aligned}
$$

For the same reason as before, the sum of the second, fourth, fifth, and seventh terms and the sum of the first, third, and sixth terms cancel out. This means, in B_6 there are no words of the form (3.23.7) (for $w_1, w_2 \geq 2,\ w_3 = 0$).
To prove the claim for $w_3 = 1$, one can use the same case distinction and obtains the results in the same way. □

3.4 Towards a q-twisted Magnus affine group scheme MQ

We will present some tentative results towards an affine group scheme corresponding to the q-twisted Magnus Lie algebra $(\mathfrak{mq}, \{-,-\}_q)$. In particular, as an analog of the twisted Magnus affine group scheme MT (Definition 3.3), we define the following.

Definition 3.24. For any commutative $\mathbb{Q}$-algebra R with unit, define

$$\mathsf{MQ}(R) = \{f \in R\langle\langle\mathcal{B}\rangle\rangle \mid (f \mid \mathbf{1}) = 1\}.$$

Here $R\langle\langle\mathcal{B}\rangle\rangle$ denotes the completion of $R\langle\mathcal{B}\rangle = \mathbb{Q}\langle\mathcal{B}\rangle \otimes R$ with respect to the weight.

Definition 3.25. Let R be a commutative $\mathbb{Q}$-algebra with unit. To all $G, H \in R\langle\langle\mathcal{B}\rangle\rangle$, assign an algebra morphism (with respect to concatenation)

$$\kappa^q_{(G,H)} : R\langle\langle\mathcal{B}\rangle\rangle \to R\langle\langle\mathcal{B}\rangle\rangle,$$

such that the following conditions hold

(i) The map $R\langle\langle\mathcal{B}\rangle\rangle \times R\langle\langle\mathcal{B}\rangle\rangle \to \mathrm{End}_R(R\langle\langle B\rangle\rangle)$, $(G,H) \mapsto \kappa^q_{(G,H)}$ is bilinear,

(ii) For all $G \in R\langle\langle\mathcal{B}\rangle\rangle$, one has

$$\kappa^q_{(\mathbf{1},G)}(\mathbf{1}) = \kappa^q_{(G,\mathbf{1})}(\mathbf{1}) = \mathbf{1}, \qquad \kappa^q_{(\mathbf{1},G)}(b_0) = \kappa^q_{(G,\mathbf{1})}(b_0) = b_0,$$

(iii) For any word $w = b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}$ in $R\langle\mathcal{B}\rangle$ and $a \geq 1$, we have

$$\kappa^q_{(\mathbf{1},w)}(b_a) = \sum_{r=0}^{k_1+\dots+k_d-d} (-1)^r \, \mathrm{lc}_1^{(a-1,r)} \circ \delta_1(b_a w),$$

$$\kappa^q_{(w,\mathbf{1})}(b_a) = \sum_{r=0}^{k_1+\dots+k_d-d} (-1)^r \, \mathrm{lc}_{d+1}^{(a-1,r)} \circ \delta_{d+1}(w b_a).$$

(iv) For all $G, H \in R\langle\langle b_0, b_1\rangle\rangle$ and $a \geq 1$, one has

$$\kappa^q_{(G,H)}(b_0) = b_0, \qquad \kappa^q_{(G,H)}(b_a) = G b_a H.$$

For two elements $G, H \in \mathsf{MQ}(R)$, we set then

$$G \circledast_q H = \kappa^q_{(G,G^{-1})}(H) G.$$

Here G^{-1} denotes the inverse with respect to the concatenation product.

Conjecture 3.26. *Let R be a commutative $\mathbb{Q}$-algebra with unit. For all $G, H \in R\langle\langle\mathcal{B}\rangle\rangle$ there are maps $\kappa^q_{(G,H)}$ satisfying the conditions in Definition 3.25, such that*

$$\mathsf{MQ} : \mathbb{Q}\text{-Alg} \to \text{Groups}, \ R \mapsto (\mathsf{MQ}(R), \circledast_q)$$

is a pro-unipotent affine group scheme.

Let $w_1 = b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}$, $w_2 = b_0^{n_0} b_{l_1} b_0^{n_1} \dots b_{l_e} b_0^{n_e}$ be words in $R\langle\mathcal{B}\rangle$ (where $k_1, \dots, k_d$, $l_1, \dots, l_e \geq 1$, $m_1, \dots, m_d, n_1, \dots, n_e \geq 0$) and $a \geq 1$, then a naive guess for the algebra morphism $\kappa_{(w_1,w_2)}$ is given by

$$\begin{aligned}
&\kappa^q_{(w_1,w_2)}(\mathbf{1}) = \mathbf{1}, \\
&\kappa^q_{(w_1,w_2)}(b_0) = b_0, \\
&\kappa^q_{(w_1,w_2)}(b_a) = \sum_{r=0}^{k_1+\dots+k_d+l_1+\dots+l_e-d-e} (-1)^r \operatorname{lc}_{d+1}^{(a-1,r)} \circ \delta_{d+1}(w_1 b_a w_2).
\end{aligned}$$

For each $\mathbb{Q}$-algebra R, let $\mathfrak{mq}(R) = \mathfrak{mq} \otimes R$ and by $\widehat{\mathfrak{mq}}(R)$ we denote the completion of $\mathfrak{mq}(R)$ with respect to the weight.

Theorem 3.27. *Assume that Conjecture 3.26 holds. Then the corresponding Lie algebra functor to the affine group scheme* MQ *is given by*

$$\widehat{\mathfrak{mq}} : \mathbb{Q}\text{-Alg} \to \text{Lie-Alg}, \ R \mapsto \left(\widehat{\mathfrak{mq}}(R), \{-,-\}_q\right).$$

Proof. It is obvious that the underlying sets of the Lie algebra functor to MQ are exactly given by the sets $\widehat{\mathfrak{mq}}(R)$ (cf Definition A.88). Thus, we are left with deriving the Lie bracket on $\widehat{\mathfrak{mq}}(R)$ from the group multiplication $\circledast_q$ on $\mathsf{MQ}(R)$. Let $G \in \mathsf{MQ}(R)$ and consider the endomorphism

$$\sigma_q(G) : R\langle\langle\mathcal{B}\rangle\rangle \to R\langle\langle\mathcal{B}\rangle\rangle, \ H \mapsto G \circledast_q H.$$

By $R[\varepsilon]$ we denote the algebra of dual numbers, so $\varepsilon^2 = 0$. For $f \in \widehat{\mathfrak{mq}}(R)$ we define the endomorphism $\tilde{s}_f : R\langle\langle\mathcal{B}\rangle\rangle \to R\langle\langle\mathcal{B}\rangle\rangle$ by

$$\sigma_q(\mathbf{1} + \varepsilon f) = \operatorname{id} + \varepsilon \tilde{s}_f.$$

Denote by $[-,-]_{\circledast_q}$ is the corresponding Lie bracket to $\circledast_q$, then we obtain

$$\tilde{s}_{[f,g]_{\circledast_q}} = [\tilde{s}_f, \tilde{s}_g], \qquad f, g \in \widehat{\mathfrak{mq}}(R). \tag{3.27.1}$$

We compute for $f \in \widehat{\mathfrak{mq}}(R)$

$$\mathbf{1} + \varepsilon f = \sigma_q(\mathbf{1} + \varepsilon f)(\mathbf{1}) = (\operatorname{id} + \varepsilon \tilde{s}_f)(\mathbf{1}) = \mathbf{1} + \varepsilon \tilde{s}_f(\mathbf{1})$$

and therefore we have $\tilde{s}_f(\mathbf{1}) = f$. So evaluating (3.27.1) in $\mathbf{1}$ we get

$$[f,g]_{\circledast_q} = \tilde{s}_f(g) - \tilde{s}_g(f), \qquad f, g \in \widehat{\mathfrak{mq}}(R). \tag{3.27.2}$$

Moreover, we define for $f \in \widehat{\mathfrak{mq}}(R)$ the endomorphism $\tilde{d}_f : R\langle\langle\mathcal{B}\rangle\rangle \to R\langle\langle\mathcal{B}\rangle\rangle$ by

$$\kappa^q_{(\mathbf{1}+\varepsilon f, (\mathbf{1}+\varepsilon f)^{-1})} = \operatorname{id} + \varepsilon \tilde{d}_f.$$

Since $\kappa^q_{(\mathbf{1}+\varepsilon f, (\mathbf{1}+\varepsilon f)^{-1})}$ is an algebra morphism by assumption, we compute for $f \in \widehat{\mathfrak{mq}}(R)$ and $u, v \in R\langle\langle\mathcal{B}\rangle\rangle$

$$\begin{aligned}
\kappa^q_{(\mathbf{1}+\varepsilon f, (\mathbf{1}+\varepsilon f)^{-1})}(uv) &= \kappa^q_{(\mathbf{1}+\varepsilon f, (\mathbf{1}+\varepsilon f)^{-1})}(u) \kappa^q_{(\mathbf{1}+\varepsilon f, (\mathbf{1}+\varepsilon f)^{-1})}(v) \\
&= (u + \varepsilon \tilde{d}_f(u))(v + \varepsilon \tilde{d}_f(v)) = uv + \varepsilon(u \tilde{d}_f(v) + \tilde{d}_f(u) v).
\end{aligned}$$

So $\tilde{d}_f$ is a derivation (for the concatenation product) and hence it suffices to obtain an explicit formula on the generators b_i, $i \geq 0$. We have for $a \geq 1$

$$\kappa^q_{(\mathbf{1}+\varepsilon f,(\mathbf{1}+\varepsilon f)^{-1})}(b_0) = \kappa^q_{(\mathbf{1}+\varepsilon f,\mathbf{1}-\varepsilon f)}(b_0) = \kappa^q_{(\mathbf{1},\mathbf{1})}(b_0) + \varepsilon\Big(\kappa^q_{(f,\mathbf{1})}(b_0) - \kappa^q_{(\mathbf{1},f)}(b_0)\Big) = b_0 + \varepsilon \cdot 0,$$
$$\kappa^q_{(\mathbf{1}+\varepsilon f,(\mathbf{1}+\varepsilon f)^{-1})}(b_a) = \kappa^q_{(\mathbf{1}+\varepsilon f,\mathbf{1}-\varepsilon f)}(b_a) = \kappa^q_{(\mathbf{1},\mathbf{1})}(b_a) + \varepsilon\Big(\kappa^q_{(f,\mathbf{1})}(b_a) - \kappa^q_{(\mathbf{1},f)}(b_a)\Big),$$

where the last equality follows from the assumption that $(G, H) \mapsto \kappa^q_{(G,H)}$ is bilinear. Thus, $\tilde{d}_f$ is the derivation determined by

$$\tilde{d}_f(b_0) = 0, \qquad \tilde{d}_f(b_a) = \kappa^q_{(f,\mathbf{1})}(b_a) - \kappa^q_{(\mathbf{1},f)}(b_a)$$

From the definition of d^q_f (Definition 3.12) and the third requirement on κ^q (Definition 3.25) we deduce that $\tilde{d}_f(b_a) = d^q_f(b_a)$ for all $a \geq 1$. In particular, we get $\tilde{d}_f = d^q_f$ for all $f \in \widehat{\mathfrak{mq}}(R)$. Finally, we calculate for $f \in \widehat{\mathfrak{mq}}(R)$ and $w \in R\langle\langle\mathcal{B}\rangle\rangle$

$$\sigma_q(\mathbf{1} + \varepsilon f)(w) = \kappa_{(\mathbf{1}+\varepsilon f,(\mathbf{1}+\varepsilon f)^{-1})}(w)(\mathbf{1} + \varepsilon f) = (w + \varepsilon d^q_f(w))(\mathbf{1} + \varepsilon f) = w + \varepsilon(wf + d^q_f(w)).$$

and therefore

$$\tilde{s}_f(w) = d^q_f(w) + wf.$$

In particular, the map $\tilde{s}_f$ equals the pre-Lie multiplication s^q_f of the q-Ihara bracket (Definition 3.16). By (3.27.2) the Lie bracket on $\widehat{\mathfrak{mq}}(R)$ is given by

$$[f, g]_{\circledast_q} = s^q_f(g) - s^q_g(f) = d^q_f(g) + gf - d^q_g(f) - fg = \{f, g\}_q,$$

where the last equality follows from the definition of the q-Ihara bracket (Definition 3.16). □

Remark 3.28. (i) Since we expect that MQ is a pro-unipotent affine group scheme with Lie algebra functor $\widehat{\mathfrak{mq}}$, there should be a natural isomorphism $\exp : \widehat{\mathfrak{mq}} \to \mathsf{MQ}$ (Theorem A.95). In particular, the q-Ihara bracket $\{-,-\}_q$ on $\widehat{\mathfrak{mq}}$ should determine the group multiplication on MQ uniquely via the Baker-Campbell-Hausdorff series. This approach to the group multiplication on MQ seems to be too extensive for this work.

(ii) In [Rac02, Section 3.1] another extension of the twisted Magnus affine group scheme MT and the twisted Magnus Lie algebra $\mathfrak{mt}$ is introduced. The product and Lie bracket in this generalization are homogeneous in depth and therefore differ significantly from the generalization given in this section.

Proposition 3.29. *Assume that Conjecture 3.26 holds. Then for each commutative $\mathbb{Q}$-algebra R with unit, there are embedding of groups*

$$\theta^{\text{anti}}_{\mathcal{X}} : (\mathsf{MT}(R), \circledast) \hookrightarrow (\mathsf{MQ}(R), \circledast_q),$$
$$x_{s_1} \ldots x_{s_l} \mapsto b_{s_l} \ldots b_{s_1}.$$

Proof. Let $G, H \in \mathsf{MT}(R)$ and recall that the algebra morphism κ_G in the group multiplication $\circledast$ is given by $\kappa_G(x_0) = x_0$, $\kappa_G(x_1) = G^{-1}x_1G$. We deduce from the condition (iv) required for κ^q (Definition 3.25) that

$$\theta^{\text{anti}}_{\mathcal{X}}(\kappa_G(H)) = \kappa^q_{(\theta^{\text{anti}}_{\mathcal{X}}(G),\theta^{\text{anti}}_{\mathcal{X}}(G)^{-1})}(\theta^{\text{anti}}_{\mathcal{X}}(H)).$$

Therefore, we get

$$\begin{aligned}\theta_{\mathcal{X}}^{\mathrm{anti}}(G \circledast H) = \theta_{\mathcal{X}}^{\mathrm{anti}}(G\kappa_G(H)) &= \theta_{\mathcal{X}}^{\mathrm{anti}}(\kappa_G(H))\theta_{\mathcal{X}}^{\mathrm{anti}}(G) \\ &= \kappa^q_{(\theta_{\mathcal{X}}^{\mathrm{anti}}(G), \theta_{\mathcal{X}}^{\mathrm{anti}}(G)^{-1})}(\theta_{\mathcal{X}}^{\mathrm{anti}}(H))\theta_{\mathcal{X}}^{\mathrm{anti}}(G) \\ &= \theta_{\mathcal{X}}^{\mathrm{anti}}(G) \circledast_q \theta_{\mathcal{X}}^{\mathrm{anti}}(H).\end{aligned}$$

□

4 Lie algebras for $\mathcal{Z}_q$: Non-commutative approach

We expect that the algebra of multiple zeta values is a free polynomial algebra decomposing into the algebra generated by $\zeta(2)$ and the graded dual of some universal enveloping algebra (Conjecture B.10). G. Racinet proved in [Rac00] that the algebra of formal multiple zeta values (Definition B.22) admits this decomposition (Corollary B.32). So assuming that the algebra of formal multiple zeta values is isomorphic to the algebra of multiple zeta values, one would obtain this decomposition for the algebra of multiple zeta values. Even more, this decomposition gives evidence for Zagier's dimension conjecture (p. 197). To show the decomposition of the algebra of formal multiple zeta values, G. Racinet introduced a pro-unipotent affine group scheme DM_0 (Definition B.24) having values in the weight-completed dual shuffle Hopf algebra (Proposition B.15) and a corresponding Lie algebra $\mathfrak{dm}_0$ (Definition B.27).
We are interested in establishing an analog approach for multiple q-zeta values. In particular, we will introduce a weight-completed Hopf algebra consisting of non-commutative power series and the algebra $\mathcal{Z}_q^f$ of formal multiple q-zeta values, whose definition is motivated by the balanced multiple q-zeta values. We will see that there is an affine scheme BM with values in this weight-completed Hopf algebra, which is represented by the algebra $\mathcal{Z}_q^f$ of formal multiple q-zeta values. This leads to the definition of a space $\mathfrak{bm}_0$, which should be seen as the dual of the space of indecomposables of $\mathcal{Z}_q^f$ (modulo the ideal generated by the formal elements $\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)$) and contains the double shuffle Lie algebra $\mathfrak{dm}_0$. We expect that $\mathfrak{bm}_0$ is a Lie subalgebra of the q-twisted Magnus Lie algebra $(\mathfrak{mq}, \{-,-\}_q)$ introduced in Subsection 3.2. Numerical experiments show that for small w the dimension of homogeneous subspaces of $\mathfrak{bm}_0$ of weight w coincide with the conjectured dimensions in 1.22 (iii). At the end of this section, we will consider the associated depth-graded space $\mathfrak{lb}$ to $\mathfrak{bm}_0$. We will show that $\mathfrak{lb}$ is properly embedded into some Lie algebra $\mathfrak{lq}$ equipped with the depth-graded q-Ihara bracket $\{-,-\}_q^D$ and we expect that $\mathfrak{lb}$ is a Lie subalgebra of $\mathfrak{lq}$. For small numbers w and d, we obtained by numerical experiments that the dimensions of the homogeneous subspaces $\mathfrak{lb}^{(w,d)}$ of weight w and depth d coincide with the dimension conjecture 1.23 (ii).

4.1 The balanced quasi-shuffle Hopf algebra

We will introduce a Hopf algebra, which should be seen as an analog of the shuffle Hopf algebra as well as the stuffle Hopf algebra for multiple zeta values (Proposition B.14, B.18). To obtain this Hopf algebra, we focus on the algebraic structure of the balanced multiple q-zeta values introduced in Subsection 2.6.

Consider the alphabet $\mathcal{B} = \{b_0, b_1, b_2, \ldots\}$, denote by $\mathcal{B}^*$ the set of all words with letters in $\mathcal{B}$, and let $\mathbf{1}$ be the empty word. For an element $b_{s_1} \ldots b_{s_l}$ in $\mathcal{B}^*$ the weight is given by

$$\mathrm{wt}(b_{s_1} \ldots b_{s_l}) = s_1 + \cdots + s_l + \#\{i \mid s_i = 0\}.$$

Equip the free non-commutative algebra $\mathbb{Q}\langle\mathcal{B}\rangle$ with the balanced quasi-shuffle product $*_q$ on $\mathbb{Q}\langle\mathcal{B}\rangle$ corresponding to (cf Definition A.52)

$$b_i \diamond_q b_j = \begin{cases} b_{i+j} & \text{if } i, j \geq 1, \\ 0 & \text{else} \end{cases}.$$

In the following, we will introduce a weight-graded Hopf algebra structure on $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q)$ and determine its completed dual.

Definition 4.1. Let $\Delta_{\text{dec}} : \mathbb{Q}\langle\mathcal{B}\rangle \to \mathbb{Q}\langle\mathcal{B}\rangle \otimes \mathbb{Q}\langle\mathcal{B}\rangle$ be the deconcatenation coproduct, so for each word $w \in \mathbb{Q}\langle\mathcal{B}\rangle$ one has

$$\Delta_{\text{dec}}(w) = \sum_{uv=w} u \otimes v.$$

Observe that the deconcatenation coproduct satisfies the recursion

$$\Delta_{\text{dec}}(b_i w) = (b_i \otimes \mathbf{1})\Delta_{\text{dec}}(w) + \mathbf{1} \otimes b_i w, \qquad b_i \in \mathcal{B},\ w \in \mathbb{Q}\langle\mathcal{B}\rangle.$$

Theorem 4.2. *The tuple $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}})$ is a weight-graded commutative Hopf algebra.*

Proof. Since $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q)$ is a quasi-shuffle algebra, this follows immediately from Theorem A.59. □

Remark 4.3. The coproduct Δ_{dec} does not preserve the space $\mathbb{Q}\langle\mathcal{B}\rangle^0$, for example we have

$$\Delta_{\text{dec}}(b_1 b_0) = \mathbf{1} \otimes b_1 b_0 + b_1 \otimes b_0 + b_1 b_0 \otimes \mathbf{1},$$

so $\mathbb{Q}\langle\mathcal{B}\rangle^0$ cannot be seen as a Hopf subalgebra of $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}})$[5].

We will give a completed dual for the Hopf algebra $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}})$ with respect to the weight. For any commutative $\mathbb{Q}$-algebra R with unit, denote $R\langle\mathcal{B}\rangle = \mathbb{Q}\langle\mathcal{B}\rangle \otimes R$ and let $R\langle\langle\mathcal{B}\rangle\rangle$ be the completion of $R\langle\mathcal{B}\rangle$ with respect to the weight (cf Proposition A.45), i.e.,

$$R\langle\langle\mathcal{B}\rangle\rangle = \prod_{w \geq 0} R\langle\mathcal{B}\rangle^{(w)},$$

where $R\langle\mathcal{B}\rangle^{(w)}$ denotes the homogeneous subspace of $R\langle\mathcal{B}\rangle$ of weight w. In particular, the elements in $R\langle\langle\mathcal{B}\rangle\rangle$ are formal non-commutative power series in the alphabet $\mathcal{B}$ with coefficients in R. The space $R\langle\langle\mathcal{B}\rangle\rangle$ is filtered by weight and depth. Similarly, denote by $R\langle\langle\mathcal{B}\rangle\rangle^0$ completion of the vector space $R\langle\mathcal{B}\rangle^0 = \mathbb{Q}\langle\mathcal{B}\rangle^0 \otimes R$.

Definition 4.4. Define the coproduct $\Delta_q : R\langle\langle\mathcal{B}\rangle\rangle \to R\langle\langle\mathcal{B}\rangle\rangle \otimes R\langle\langle\mathcal{B}\rangle\rangle$ by

$$\Delta_q(b_i) = \mathbf{1} \otimes b_i + b_i \otimes \mathbf{1} + \sum_{j=1}^{i-1} b_j \otimes b_{i-j}, \qquad i \geq 0.$$

and extend this definition with respect to the concatenation product.

Theorem 4.5. *The tuple $(R\langle\langle\mathcal{B}\rangle\rangle, \text{conc}, \Delta_q)$ is a complete cocommutative Hopf algebra. The pairing*

$$R\langle\langle\mathcal{B}\rangle\rangle \otimes \mathbb{Q}\langle\mathcal{B}\rangle \to R,$$
$$\Phi \otimes w \mapsto (\Phi \mid w),$$

where $(\Phi \mid w)$ denotes the coefficient of w in Φ, gives a duality between the weight-graded Hopf algebra $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}})$ and the complete Hopf algebra $(R\langle\langle\mathcal{B}\rangle\rangle, \text{conc}, \Delta_q)$.

[5] After the submission of this thesis a regularized coproduct $\mathbb{Q}\langle\mathcal{B}\rangle^0$ is obtained, which endows $(\mathbb{Q}\langle\mathcal{B}\rangle^0, *_q)$ with a Hopf algebra structure (ArXiv: 2303.09436 [math.NT]).

Proof. We prove the duality of $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}})$ and $(R\langle\langle\mathcal{B}\rangle\rangle, \text{conc}, \Delta_q)$ with respect to the given pairing. Then $(R\langle\langle\mathcal{B}\rangle\rangle, \text{conc}, \Delta_q)$ is a cocommutative Hopf algebra (Theorem A.31). It is well-known that Δ_{dec} and conc are dual maps. Moreover, for $u, v \in \mathbb{Q}\langle\mathcal{B}\rangle$ one obtains

$$(\Delta_q(b_i) \mid u \otimes v) = \Big(\mathbf{1} \otimes b_i + b_i \otimes \mathbf{1} + \sum_{j=1}^{i-1} b_i \otimes b_{i-j} \Bigm| u \otimes v\Big) = (b_i \mid u *_q v)$$

The last equality holds, since the word b_i appears in the product $u *_q v$ if and only if $u = \mathbf{1},\ v = b_i$ or $u = b_i,\ v = \mathbf{1}$ or $u = b_j,\ v = b_{i-j}$ for some $j = 1, \dots, i-1$. Since Δ_q is compatible with the concatenation product by definition and the letters b_i generate the algebra $(R\langle\langle\mathcal{B}\rangle\rangle, \text{conc})$, we deduce that the maps Δ_q and $*_q$ are dual. □

Remark 4.6. The coproduct Δ_q does not preserve the space $R\langle\langle\mathcal{B}\rangle\rangle^0$, for example we have

$$\Delta_q(b_1 b_0) = b_1 b_0 \otimes \mathbf{1} + b_1 \otimes b_0 + b_0 \otimes b_1 + \mathbf{1} \otimes b_1 b_0.$$

Lemma 4.7. *The antipode S_q of $(R\langle\langle\mathcal{B}\rangle\rangle, \text{conc}, \Delta_q)$ is the anti-automorphism defined by*

$$\begin{aligned} S_q(b_0) &= -b_0, \\ S_q(b_a) &= \sum_{r=1}^{a} \sum_{\substack{j_1+\dots+j_r=a \\ j_1,\dots,j_r \geq 1}} (-1)^r b_{j_1} \dots b_{j_r}, \qquad a \geq 1. \end{aligned}$$

Proof. The letter b_0 is primitive for the coproduct Δ_q, thus we deduce from Theorem A.38 (ii) that $S_q(b_0) = -b_0$. Moreover, compute for $a \geq 1$

$$\begin{aligned} \Big(\text{conc} \circ (S_q \otimes \text{id}) \circ \Delta_q\Big)(b_a) &= S_q(\mathbf{1}) \cdot b_a + S_q(b_a) \cdot \mathbf{1} + \sum_{n=1}^{a-1} S_q(b_n) \cdot b_{a-n} \\ &= b_a + \sum_{r=1}^{a} \sum_{\substack{j_1+\dots+j_r=a \\ j_1,\dots,j_r \geq 1}} (-1)^r b_{j_1} \dots b_{j_r} + \sum_{n=1}^{a-1} \sum_{s=1}^{n} \sum_{\substack{i_1+\dots+i_s=n \\ i_1,\dots,i_s \geq 1}} (-1)^s b_{i_1} \dots b_{i_s} b_{a-n} \\ &= \sum_{r=2}^{a} \sum_{\substack{j_1+\dots+j_r=a \\ j_1,\dots,j_r \geq 1}} (-1)^r b_{j_1} \dots b_{j_r} + \sum_{s=1}^{a-1} \sum_{\substack{i_1+\dots+i_{s+1}=a \\ i_1,\dots,i_{s+1} \geq 1}} (-1)^s b_{i_1} \dots b_{i_{s+1}} \\ &= 0 = \varepsilon(b_a) \end{aligned}$$

and similarly one checks

$$\Big(\text{conc} \circ (\text{id} \otimes S_q) \circ \Delta_q\Big)(b_a) = 0 = \varepsilon(b_a), \qquad a \geq 1.$$

□

Relation to the Hopf algebras of multiple zeta values. Consider the shuffle Hopf algebra $(\mathbb{Q}\langle\mathcal{X}\rangle, ш, \Delta_{\text{dec}})$ (Proposition B.14) and the stuffle Hopf algebra $(\mathbb{Q}\langle\mathcal{Y}\rangle, *, \Delta_{\text{dec}})$ (Proposition B.18) defined within the context of multiple zeta values. Both of them are closely related to the balanced quasi-shuffle Hopf algebra $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}})$, more precisely there are two surjective Hopf algebra morphisms

$$\begin{aligned} (\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}}) &\twoheadrightarrow (\mathbb{Q}\langle\mathcal{X}\rangle, ш, \Delta_{\text{dec}}), \\ b_0 &\mapsto x_0, \\ b_1 &\mapsto x_1, \\ b_i &\mapsto 0, \quad i \geq 2 \end{aligned}$$

and

$$(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}}) \twoheadrightarrow (\mathbb{Q}\langle\mathcal{Y}\rangle, *, \Delta_{\mathrm{dec}}),$$
$$b_0 \mapsto 0$$
$$b_i \mapsto y_i, \quad i \geq 1.$$

By duality, we also obtain two injective Hopf algebra morphisms

$$\theta_{\mathcal{X}} : (R\langle\langle\mathcal{X}\rangle\rangle, \mathrm{conc}, \Delta_{\sqcup\!\sqcup}) \hookrightarrow (R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q), \qquad (4.7.1)$$
$$x_0 \mapsto b_0,$$
$$x_1 \mapsto b_1,$$

and

$$\theta_{\mathcal{Y}} : (R\langle\langle\mathcal{Y}\rangle\rangle, \mathrm{conc}, \Delta_*) \hookrightarrow (R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q), \qquad (4.7.2)$$
$$y_i \mapsto b_i, \quad i \geq 1.$$

Remark 4.8. The stuffle Hopf algebra $(\mathbb{Q}\langle\mathcal{Y}\rangle, *, \Delta_{\mathrm{dec}})$ can be identified with the Hopf subalgebra of $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}})$ spanned by all words, which do not contain the letter b_0. This leads to an injective Hopf algebra morphism

$$(\mathbb{Q}\langle\mathcal{Y}\rangle, *, \Delta_{\mathrm{dec}}) \hookrightarrow (\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}}),$$
$$y_i \mapsto b_i, \quad i \geq 1.$$

On the other hand, we have $b_1 *_q b_1 = 2b_1^2 + b_2$, and thus the words containing only the letters b_0, b_1 do not span a Hopf subalgebra of $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}})$. Therefore the shuffle Hopf algebra $(\mathbb{Q}\langle\mathcal{X}\rangle, \sqcup\!\sqcup, \Delta_{\mathrm{dec}})$ does not canonically embed into $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}})$. In particular, one obtains a sequence of Hopf algebras

$$0 \to (\mathbb{Q}\langle\mathcal{Y}\rangle, *, \Delta_{\mathrm{dec}}) \hookrightarrow (\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}}) \twoheadrightarrow (\mathbb{Q}\langle\mathcal{X}\rangle, \sqcup\!\sqcup, \Delta_{\mathrm{dec}}) \to 0, \qquad (4.8.1)$$

which is nearly exact (the only exception is the span of the words $b_1^n \in \mathbb{Q}\langle\mathcal{B}\rangle$, $n \geq 0$).

4.2 Regularized multiple q-zeta values

Let $\mathbb{Q}\langle\mathcal{B}\rangle^0$ be the subalgebra of $\mathbb{Q}\langle\mathcal{B}\rangle$ generated by all words, which do not start with b_0. Then the involution $\tau : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q}\langle\mathcal{B}\rangle^0$ is given by $\tau(\mathbf{1}) = \mathbf{1}$ and

$$\tau(b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d}) = b_{m_d+1}b_0^{k_d-1}\dots b_{m_1+1}b_0^{k_1-1}. \tag{4.8.2}$$

By Theorem 2.59 we have a surjective τ-invariant algebra morphism

$$\begin{aligned}\zeta_q : (\mathbb{Q}\langle\mathcal{B}\rangle^0, *_q) &\to (\mathcal{Z}_q, \cdot), \\ b_{s_1}\dots b_{s_l} &\mapsto \zeta_q(s_1,\dots,s_l).\end{aligned} \tag{4.8.3}$$

On the other hand, we introduced the balanced quasi-shuffle Hopf algebra $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}})$ and observed that the coproduct Δ_{dec} cannot be restricted to the subalgebra $\mathbb{Q}\langle\mathcal{B}\rangle^0$ or respectively the dual coproduct Δ_q to $R\langle\langle\mathcal{B}\rangle\rangle^0$ (Remark 4.3, 4.6). So to define an algebra of formal multiple q-zeta values analogues to $\mathcal{Z}^f$ (Definition B.22), we need to extend the algebra morphism given in (4.8.3) to the whole algebra $\mathbb{Q}\langle\mathcal{B}\rangle$. This will yield the definition of regularized multiple q-zeta values.

Proposition 4.9. *Let T be a formal variable and extend the product $*_q$ by $\mathbb{Q}[T]$-linearity to $\mathbb{Q}\langle\mathcal{B}\rangle^0[T]$. The map*

$$\begin{aligned}\operatorname{reg}_q :\ \mathbb{Q}\langle\mathcal{B}\rangle^0[T] &\to \mathbb{Q}\langle\mathcal{B}\rangle, \\ wT^n &\mapsto w *_q b_0^{*_q n}\end{aligned}$$

is an algebra isomorphism for the balanced quasi-shuffle product $*_q$.

Proof. For the surjectivity of reg_q, we show that any word $w \in \mathbb{Q}\langle\mathcal{B}\rangle$ is a polynomial in b_0 with coefficients in $\mathbb{Q}\langle\mathcal{B}\rangle^0$. Let $w = b_0^{m_0}b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d}$ for some integers $k_1,\dots,k_d \geq 1$ and $m_0,\dots,m_d \geq 0$. We prove by induction on m_0, that $w = u + v *_q b_0$ for some $u \in \mathbb{Q}\langle\mathcal{B}\rangle^0$ and $v \in \mathbb{Q}\langle\mathcal{B}\rangle$, where all words in v have weight $< \operatorname{wt}(w)$. Then induction on the weight proves the claim. The case $m_0 = 0$ is trivial, simply choose $u = w,\ v = 0$. Next, calculate

$$\begin{aligned}b_0^{m_0-1}b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d} *_q b_0 &= m_0\ b_0^{m_0}b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d} \\ &\quad+ \sum_{i=1}^{d}(m_i+1)\ b_0^{m_0-1}b_{k_1}b_0^{m_1}\dots b_{k_i}b_0^{m_i+1}b_{k_{i+1}}b_0^{m_{i+1}}\dots b_{k_d}b_0^{m_d}.\end{aligned}$$

Applying the induction hypotheses to every word in the second line leads to

$$w = \frac{1}{m_0}\Big(u + (v + b_0^{m_0-1}b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d}) *_q b_0\Big)$$

for some $u \in \mathbb{Q}\langle\mathcal{B}\rangle^0$ and $v \in \mathbb{Q}\langle\mathcal{B}\rangle$, where $v + b_0^{m_0-1}b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d}$ consists of words of weight $< \operatorname{wt}(w)$.
Let $P \in \mathbb{Q}\langle\mathcal{B}\rangle^0[T]\backslash\{0\}$ and write $P = wT^n + R$, where $w \in \mathbb{Q}\langle\mathcal{B}\rangle^0\backslash\{0\}$ and $R \in \mathbb{Q}\langle\mathcal{B}\rangle^0[T]$ is a polynomial of degree $< n$. We have

$$\operatorname{reg}_q(P) = w *_q b_0^{*_q n} + \operatorname{reg}_q(R) = n!b_0^n w + \widetilde{w},$$

where $\widetilde{w} \in \mathbb{Q}\langle\mathcal{B}\rangle$ consists of words with at most $(n-1)$-times the letter b_0 at the beginning. We deduce $\operatorname{reg}_q(P) \neq 0$, thus reg_q is injective. $\square$

Definition 4.10. For every $w \in \mathbb{Q}\langle\mathcal{B}\rangle$, define the regularized multiple q-zeta values by

$$\zeta_q^{\text{reg}}(w) = \zeta_q\Big(\operatorname{reg}_q^{-1}(w)|_{T=0}\Big).$$

This definition is unique in the following sense.

Theorem 4.11. *The map* $\zeta_q^{\mathrm{reg}} : \mathbb{Q}\langle\mathcal{B}\rangle \to \mathcal{Z}_q,\ w \mapsto \zeta_q^{\mathrm{reg}}(w)$ *is the only map satisfying*

$$\begin{array}{lrcll} \text{(i)} & \zeta_q^{\mathrm{reg}}(w) & = & \zeta_q(w) & w \in \mathbb{Q}\langle\mathcal{B}\rangle^0, \\ \text{(ii)} & \zeta_q^{\mathrm{reg}}(b_0) & = & 0, & \\ \text{(iii)} & \zeta_q^{\mathrm{reg}}(v *_q w) & = & \zeta_q^{\mathrm{reg}}(v)\zeta_q^{\mathrm{reg}}(w), & v, w \in \mathbb{Q}\langle\mathcal{B}\rangle. \end{array}$$

Proof. Since reg_q is the identity on $\mathbb{Q}\langle\mathcal{B}\rangle^0$, the map ζ_q^{reg} satisfies (i). Moreover, we have $(\mathrm{reg}_q)^{-1}(b_0) = T$ and thus $\zeta_q^{\mathrm{reg}}(b_0) = 0$. Finally, reg_q is an algebra isomorphism for $*_q$, hence ζ_q^{reg} satisfies (iii).
By Proposition 4.9, any word $w \in \mathbb{Q}\langle\mathcal{B}\rangle$ is a polynomial in b_0 with coefficients in $\mathbb{Q}\langle\mathcal{B}\rangle^0$. Thus any algebra morphism on $\mathbb{Q}\langle\mathcal{B}\rangle$ (with respect to the product $*_q$) is uniquely determined by its values on b_0 and words in $\mathbb{Q}\langle\mathcal{B}\rangle^0$. □

Note that the map τ is only defined on the space $\mathbb{Q}\langle\mathcal{B}\rangle^0$ (cf (4.8.2)) and not on $\mathbb{Q}\langle\mathcal{B}\rangle$, thus we cannot require all regularized multiple q-zeta values to be τ-invariant.

4.3 Formal multiple q-zeta values

Similar to the case of multiple zeta values ([IKZ06], [Ec02]), we want to formalize the algebraic relations satisfied in the algebra $\mathcal{Z}_q$. To describe them we use the spanning set given by the balanced multiple q-zeta values $\zeta_q(s_1,\dots,s_l)$, $s_1 \geq 1$, $s_2,\dots,s_l \geq 0$. Their description in terms of the alphabet $\mathcal{B}$ allows to connect the formal multiple q-zeta values to Hopf algebra structures closely related to the ones of multiple zeta values (given in [Rac00]).

In (4.8.3) we have seen that there is a τ-invariant surjective algebra morphism

$$\begin{aligned}\zeta_q : (\mathbb{Q}\langle\mathcal{B}\rangle^0, *_q) &\to (\mathcal{Z}_q, \cdot),\\ b_{s_1}\dots b_{s_l} &\mapsto \zeta_q(s_1,\dots,s_l).\end{aligned}$$

We expect that all algebraic relations in $\mathcal{Z}_q$ are encoded in this morphism, which means that all relations in $\mathcal{Z}_q$ should be a consequence of the balanced quasi-shuffle product formula and the τ-invariance of the balanced multiple q-zeta values (Conjecture 2.60). This will determine the definition of the algebra of formal multiple q-zeta values. In order to link the algebra of formal multiple q-zeta values to the Hopf algebra structures introduced in Subsection 4.1, we will use instead the extended map

$$\begin{aligned}\zeta_q : (\mathbb{Q}\langle\mathcal{B}\rangle, *_q) &\to (\mathcal{Z}_q, \cdot),\\ b_{s_1}\dots b_{s_l} &\mapsto \zeta_q^{\mathrm{reg}}(s_1,\dots,s_l),\end{aligned}$$

which is by Theorem 4.11 completely determined by the balanced multiple q-zeta values.

Definition 4.12. The algebra $\mathcal{Z}_q^f$ of formal multiple q-zeta values[6] is given by

$$\mathcal{Z}_q^f = {(\mathbb{Q}\langle\mathcal{B}\rangle, *_q)}\big/{\mathrm{Rel_q}},$$

where $\mathrm{Rel_q}$ is the ideal in $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q)$ generated by $\{b_0\} \cup \{w - \tau(w) \mid w \in \mathbb{Q}\langle\mathcal{B}\rangle^0\}$.

Denote by $\zeta_q^f(w)$ the image of $w \in \mathbb{Q}\langle\mathcal{B}\rangle$ in the quotient space $\mathcal{Z}_q^f$ and set $\zeta_q^f(\mathbf{1}) = 1$. Then $\mathcal{Z}_q^f$ is the weight-graded algebra spanned by the elements $\zeta_q^f(w)$, $w \in \mathcal{B}^*$, which exactly satisfy the following relations

$$\begin{array}{llcll}\text{(i)} & \zeta_q^f(b_0) & = & 0 & \\ \text{(ii)} & \zeta_q^f(v *_q w) & = & \zeta_q^f(v)\zeta_q^f(w), & v,w \in \mathbb{Q}\langle\mathcal{B}\rangle \\ \text{(iii)} & \zeta_q^f(\tau(w)) & = & \zeta_q^f(w), & w \in \mathbb{Q}\langle\mathcal{B}\rangle^0\end{array}$$

Observe that we have similar to Theorem 4.11)

$$\zeta_q^f(w) = \zeta_q^f\Big(\mathrm{reg}_q^{-1}(w)|_{T=0}\Big) \quad \text{for all } w \in \mathbb{Q}\langle\mathcal{B}\rangle.$$

Thus, the space $\mathcal{Z}_q^f$ is spanned by the elements $\zeta_q^f(w)$, where $w \in \mathbb{Q}\langle\mathcal{B}\rangle^0$ are words.

Remark 4.13. In [BIM] the algebra of formal multiple Eisenstein series is studied, which is isomorphic to the algebra $\mathcal{Z}_q^f$ (on the level of generating series the isomorphism is given by $\#_Y$, cf Theorem 2.75).

[6] A more precise name would be formal regularized balanced multiple q-zeta values, but for simplicity we call them just formal multiple q-zeta values. The notation of this space might change in forthcoming work, because it is also related to multiple Eisenstein series.

By definition, the algebra $\mathcal{Z}_q^f$ is equipped with the following universal property.

Proposition 4.14. *For every $\mathbb{Q}$-algebra R and every algebra morphism*

$$\varphi : (\mathbb{Q}\langle \mathcal{B} \rangle, *_q) \to R,$$

which is τ-invariant on $\mathbb{Q}\langle \mathcal{B} \rangle^0$ and satisfies $\varphi(b_0) = 0$, there exists a unique algebra morphism $\widetilde{\varphi} : \mathcal{Z}_q^f \to R$, such that the following diagram commutes

$$\begin{array}{ccc} \mathbb{Q}\langle \mathcal{B} \rangle & \xrightarrow{\zeta_q^f} & \mathcal{Z}_q^f \\ & \searrow^{\varphi} & \downarrow{\scriptstyle \widetilde{\varphi}} \\ & & R \end{array}$$

Corollary 4.15. *There is a surjective algebra morphism*

$$\mathcal{Z}_q^f \twoheadrightarrow \mathcal{Z}_q,$$
$$\zeta_q^f(w) \mapsto \zeta_q^{\mathrm{reg}}(w).$$

Proof. By Theorem 4.11, the map $\mathbb{Q}\langle \mathcal{B} \rangle \to \mathcal{Z}_q,\ w \mapsto \zeta_q^{\mathrm{reg}}(w)$ is an algebra morphism satisfying $\zeta_q^{\mathrm{reg}}(b_0) = 0$. Moreover, for each $w \in \mathbb{Q}\langle \mathcal{B} \rangle^0$ one has $\zeta_q^{\mathrm{reg}}(w) = \zeta_q(w)$ and the balanced multiple zeta values are τ-invariant on $\mathbb{Q}\langle \mathcal{B} \rangle^0$ (Theorem 2.59). Therefore, we can apply Proposition 4.14 to the map $\mathbb{Q}\langle \mathcal{B} \rangle \to \mathcal{Z}_q,\ w \mapsto \zeta_q^{\mathrm{reg}}(w)$ and obtain an algebra morphism

$$\mathcal{Z}_q^f \to \mathcal{Z}_q,\ \zeta_q^f(w) \mapsto \zeta_q^{\mathrm{reg}}(w).$$

Since the balanced multiple q-zeta values form a spanning set of $\mathcal{Z}_q$ (Proposition 2.57), one obtains surjectivity. □

All relations in $\mathcal{Z}_q$ should be induced by the balanced quasi-shuffle product formula and the τ-invariance of the balanced multiple q-zeta values (Conjecture 2.60), therefore we expect that the morphism in Corollary 4.15 is an isomorphism.

Corollary 4.16. *The elements $\zeta_q^f(2),\ \zeta_q^f(4),\ \zeta_q^f(6)$ are algebraic independent. In particular, $\mathbb{Q}[\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)]$ is a free polynomial algebra isomorphic to the algebra $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$ of quasi-modular forms.*

Proof. The balanced multiple q-zeta values $\zeta_q(2),\ \zeta_q(4),\ \zeta_q(6)$ equal the classical Eisenstein series of weight $2, 4, 6$ (Example 2.61 2)). Thus, we obtain from classical results in the theory of quasi-modular forms that $\zeta_q(2),\ \zeta_q(4),\ \zeta_q(6)$ are algebraic independent and that $\mathbb{Q}[\zeta_q(2), \zeta_q(4), \zeta_q(6)]$ is a free polynomial algebra equal to the algebra $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$ ([MR05, Lemma 117, Proposition 124]). Since we have by Corollary 4.15 a surjective algebra morphism $\mathcal{Z}_q^f \to \mathcal{Z}_q$ sending $\zeta_q^f(k)$ to $\zeta_q(k)$ for each $k \geq 1$, we deduce that also the elements $\zeta_q^f(2),\ \zeta_q^f(4),\ \zeta_q^f(6)$ are algebraic independent and that the free polynomial algebra $\mathbb{Q}[\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)]$ is isomorphic to $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$. □

Similar to the case of multiple zeta values ([Rac00]), we want to relate the algebra $\mathcal{Z}_q^f$ to a subset of the Hopf algebra $(R\langle\langle \mathcal{B} \rangle\rangle, \mathrm{conc}, \Delta_q)$.

Definition 4.17. For each commutative $\mathbb{Q}$-algebra R with unit, denote by $\mathsf{BM}(R)$ the set of all non-commutative power series Φ in $R\langle\langle \mathcal{B} \rangle\rangle$ satisfying

$$\begin{array}{lccc} \text{(i)} & (\Phi|b_0) & = & 0, \\ \text{(ii)} & \Delta_q(\Phi) & = & \Phi\hat{\otimes}\Phi, \\ \text{(iii)} & \tau(\Pi_0(\Phi)) & = & \Pi_0(\Phi). \end{array}$$

Here Π_0 denotes the R-linear extension of the canonical projection $\mathbb{Q}\langle\mathcal{B}\rangle \to \mathbb{Q}\langle\mathcal{B}\rangle^0$, which is the identity on $\mathbb{Q}\langle\mathcal{B}\rangle^0$ and maps all words starting with b_0 to 0.

For each $\lambda_1, \lambda_2, \lambda_3 \in R$, let $\mathsf{BM}_{(\lambda_1,\lambda_2,\lambda_3)}(R)$ be the subset of all $\Phi \in \mathsf{BM}(R)$ additionally satisfying

$$\text{(iv)}\quad (\Phi \mid b_2) = \lambda_1, \qquad (\Phi \mid b_4) = \lambda_2, \qquad (\Phi \mid b_6) = \lambda_3.$$

We abbreviate $\mathsf{BM}_0(R) = \mathsf{BM}_{(0,0,0)}(R)$.

Theorem 4.18. *For every commutative $\mathbb{Q}$-algebra R with unit, there are bijections*

$$\mathsf{BM}(R) \simeq \mathrm{Hom}_{\mathbb{Q}\text{-Alg}}(\mathcal{Z}_q^f, R), \qquad \mathsf{BM}_0(R) \simeq \mathrm{Hom}_{\mathbb{Q}\text{-Alg}}\left(\mathcal{Z}_q^f \big/ \big(\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)\big), R \right).$$

In particular, $\mathsf{BM} : \mathbb{Q}\text{-Alg} \to \text{Sets}$ *is an affine scheme represented by the algebra* $\mathcal{Z}_q^f$ *and* $\mathsf{BM}_0 : \mathbb{Q}\text{-Alg} \to \text{Sets}$ *is an affine scheme represented by* $\mathcal{Z}_q^f \big/ \big(\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)\big)$.

An introduction to affine (group) schemes is given in Appendix A.6. Note that for these bijections the regularization in Theorem 4.11 is essential.

Proof. The first bijection is given by the map

$$\begin{aligned} f : \mathrm{Hom}_{\mathbb{Q}\text{-Alg}}(\mathcal{Z}_q^f, R) &\to \mathsf{BM}(R), \\ \varphi &\mapsto \sum_{w \in \mathcal{B}^*} \varphi(\zeta_q^f(w))w. \end{aligned}$$

Let $\varphi : \mathcal{Z}_q^f \to R$ be a $\mathbb{Q}$-algebra morphism. Since $\zeta_q^f(b_0) = 0$, we obtain $(f(\varphi)|b_0) = 0$. The formal multiple q-zeta values satisfy the balanced quasi-shuffle product formula, thus we have $(f(\varphi)|u *_q v) = (f(\varphi)|u)(f(\varphi)|v)$ for all $u, v \in \mathbb{Q}\langle\mathcal{B}\rangle$. From the duality of $*_q$ and Δ_q (Theorem 4.5), we deduce

$$(\Delta_q(f(\varphi)) \mid u \otimes v) = (f(\varphi) \mid u *_q v) = (f(\varphi) \mid u)\ (f(\varphi) \mid v) = (f(\varphi) \otimes f(\varphi) \mid u \otimes v)$$

for all $u, v \in \mathbb{Q}\langle\mathcal{B}\rangle$. In particular, the power series $f(\varphi)$ is grouplike for Δ_q. Since τ maps words onto words, the τ-invariance of the formal multiple q-zeta values on $\mathbb{Q}\langle\mathcal{B}\rangle^0$ implies $\tau\big(\Pi_0(f(\varphi))\big) = \Pi_0(f(\varphi))$. This shows that $\varphi(f)$ is contained in the set $\mathsf{BM}(R)$ and therefore the map f is well-defined. The inverse of f is given by

$$\begin{aligned} \mathsf{BM}(R) &\to \mathrm{Hom}_{\mathbb{Q}\text{-Alg}}(\mathcal{Z}_q^f, R), \\ \Phi &\mapsto \Big(\zeta_q^f(w) \mapsto (\Phi \mid w)\Big), \end{aligned}$$

hence f is indeed a bijection. It is an immediate consequence that f also induces a bijection

$$\begin{aligned} \Big\{\varphi \in \mathrm{Hom}_{\mathbb{Q}\text{-Alg}}(\mathcal{Z}_q^f, R) \;\Big|\; \varphi(\zeta_q^f(2)) = \varphi(\zeta_q^f(4)) = \varphi(\zeta_q^f(6)) = 0\Big\} &\to \mathsf{BM}_0(R), \\ \varphi &\mapsto f(\varphi). \end{aligned}$$

By the universal property of the quotient space, the set on the left hand side is in bijection to

$$\mathrm{Hom}_{\mathbb{Q}\text{-Alg}}\left(\mathcal{Z}_q^f \big/ \big(\zeta_q^f(2), \zeta_q^f(4), \zeta_q^f(6)\big), R \right).$$

This yields the second claimed isomorphy. $\square$

Corollary 4.19. *For the regularized multiple q-zeta values given in Definition 4.10, one obtains*

$$\sum_{w\in\mathcal{B}^*} \zeta_q^{\mathrm{reg}}(w)w \in \mathsf{BM}(\mathcal{Z}_q).$$

Proof. Apply the bijection in Theorem 4.18 to the $\mathbb{Q}$-algebra morphism

$$\mathcal{Z}_q^f \to \mathcal{Z}_q,\ \zeta_q^f(w) \mapsto \zeta_q^{\mathrm{reg}}(w)$$

given in Corollary 4.15. □

Relation between formal multiple q-zeta values and formal multiple zeta values. Let R be a commutative $\mathbb{Q}$-algebra with unit. We relate the set $\mathsf{DM}(R)$ defined for multiple zeta values (Definition B.24) to the set $\mathsf{BM}(R)$. This leads to a projection from the algebra $\mathcal{Z}_q^f$ of formal multiple q-zeta values onto the algebra $\mathcal{Z}^f$ of formal multiple zeta values (Definition B.22). We will need the embeddings of the dual shuffle and stuffle Hopf algebra into $(R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q)$, those were defined in (4.7.1) and (4.7.2) as

$$\begin{aligned}\theta_{\mathcal{X}} &: (R\langle\langle\mathcal{X}\rangle\rangle, \mathrm{conc}, \Delta_{\sqcup\!\sqcup}) \to (R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q),\ x_i \mapsto b_i \quad (i\in\{0,1\})\\ \theta_{\mathcal{Y}} &: \ (R\langle\langle\mathcal{Y}\rangle\rangle, \mathrm{conc}, \Delta_*) \to (R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q),\ y_i \mapsto b_i \quad (i\geq 1).\end{aligned}$$

To capture the fact that the map τ is an anti-morphism, we consider the following Hopf algebra anti morphism

$$\begin{aligned}\theta_{\mathcal{X}}^{\mathrm{anti}} : (R\langle\langle\mathcal{X}\rangle\rangle, \mathrm{conc}, \Delta_{\sqcup\!\sqcup}) &\to (R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q),\\ x_{s_1}\ldots x_{s_l} &\mapsto b_{s_l}\ldots b_{s_1}.\end{aligned} \tag{4.19.1}$$

Lemma 4.20. *For the canonical projections* $\Pi_0 : R\langle\langle\mathcal{B}\rangle\rangle \to R\langle\langle\mathcal{B}\rangle\rangle^0$ *(Definition 4.17) and* $\Pi_{\mathcal{Y}} : R\langle\langle\mathcal{X}\rangle\rangle \to R\langle\langle\mathcal{Y}\rangle\rangle$ *(Definition B.24), we have*

$$\tau\circ\Pi_0\circ\theta_{\mathcal{X}}^{\mathrm{anti}} = \theta_{\mathcal{Y}}\circ\Pi_{\mathcal{Y}}.$$

Proof. For a word $w = x_0^{k_1-1}x_1\ldots x_0^{k_d-1}x_1$ in $R\langle\langle\mathcal{X}\rangle\rangle$ (where $k_1,\ldots,k_d\geq 1$), we compute

$$(\tau\circ\Pi_0\circ\theta_{\mathcal{X}}^{\mathrm{anti}})(w) = \tau(b_1b_0^{k_d-1}\ldots b_1b_0^{k_1-1}) = b_{k_1}\ldots b_{k_d} = \theta_{\mathcal{Y}}(y_{k_1}\ldots y_{k_d}) = (\theta_{\mathcal{Y}}\circ\Pi_{\mathcal{Y}})(w).$$

If $w = vx_0$ for some word v in $R\langle\langle\mathcal{X}\rangle\rangle$, we obtain

$$(\tau\circ\Pi_0\circ\theta_{\mathcal{X}}^{\mathrm{anti}})(w) = (\tau\circ\Pi_0)(b_0\theta_{\mathcal{X}}^{\mathrm{anti}}(v)) = 0 = \Pi_{\mathcal{Y}}(vx_0) = (\theta_{\mathcal{Y}}\circ\Pi_{\mathcal{Y}})(w)$$

□

Theorem 4.21. *For each commutative* $\mathbb{Q}$*-algebra* R *with unit, we have an injective map*

$$\begin{aligned}\theta : \mathsf{DM}(R) &\to \mathsf{BM}(R),\\ \phi &\mapsto \theta_{\mathcal{X}}^{\mathrm{anti}}(\phi)\theta_{\mathcal{Y}}(\phi_*)\end{aligned}$$

where we denote (as in Definition B.24)

$$\phi_* = \phi_{\mathrm{corr}}\Pi_{\mathcal{Y}}(\phi) = \exp\left(\sum_{n\geq 2}\frac{(-1)^{n-1}}{n}(\Pi_{\mathcal{Y}}(\phi)|y_n)y_1^n\right)\Pi_{\mathcal{Y}}(\phi) \in R\langle\langle\mathcal{Y}\rangle\rangle.$$

The chosen order of the factors in the definition of θ is necessary for the compatibility of the projections $\Pi_{\mathcal{Y}}$ and Π_0 under the map θ.

Proof. Let $\phi \in \mathsf{DM}(R)$. We have $(\phi \mid x_0) = 0$ and hence $(\theta(\phi) \mid b_0) = 0$. Since $\theta_{\mathcal{X}}^{\mathrm{anti}}$, $\theta_{\mathcal{Y}}$ are coalgebra morphisms and ϕ and ϕ_* are grouplike for $\Delta_{⧢}$ and Δ_*, we compute

$$\begin{aligned}\Delta_q(\theta(\phi)) &= \Delta_q(\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi))\Delta_q(\theta_{\mathcal{Y}}(\phi_*)) = (\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi) \hat{\otimes} \theta_{\mathcal{X}}^{\mathrm{anti}}(\phi))(\theta_{\mathcal{Y}}(\phi_*) \hat{\otimes} \theta_{\mathcal{Y}}(\phi_*)) \\ &= \theta(\phi) \hat{\otimes} \theta(\phi).\end{aligned}$$

By Lemma 4.20, we obtain

$$\begin{aligned}\tau\Big(\Pi_0(\theta(\phi))\Big) &= \tau\Big(\Pi_0(\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi))\theta_{\mathcal{Y}}(\phi_*)\Big) = \tau\Big(\theta_{\mathcal{Y}}(\phi_*)\Big)\tau\Big(\Pi_0(\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi))\Big) \\ &= \tau\Big(\theta_{\mathcal{Y}}(\phi_*)\Big)\theta_{\mathcal{Y}}\Big(\Pi_{\mathcal{Y}}(\phi)\Big) = \tau\Big(\theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\phi))\Big)\tau\Big(\theta_{\mathcal{Y}}(\phi_{\mathrm{corr}})\Big)\theta_{\mathcal{Y}}\Big(\Pi_{\mathcal{Y}}(\phi)\Big) \\ &= \Pi_0\Big(\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi)\Big)\theta_{\mathcal{Y}}\Big(\phi_{\mathrm{corr}}\Big)\theta_{\mathcal{Y}}\Big(\Pi_{\mathcal{Y}}(\phi)\Big) = \Pi_0\Big(\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi)\Big)\theta_{\mathcal{Y}}(\phi_*) \\ &= \Pi_0\Big(\theta(\phi)\Big).\end{aligned}$$

Note that $\theta_{\mathcal{Y}}(\phi_{\mathrm{corr}})$ consists of the letter b_1 and is therefore τ-invariant. We have proven that $\theta(\phi)$ is an element in $\mathsf{BM}(R)$ and thus the map θ is well-defined.
Next, we show injectivity. The elements $\phi \in \mathsf{DM}(R)$ satisfy $(\phi \mid x_1) = 0$ and hence also $(\phi \mid x_1^n) = 0$ for all $n \geq 1$. Thus, any non-trivial word in $\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi)$ contains the letter b_0 and every non-trivial word in $\theta_{\mathcal{Y}}(\phi_*)$ contains a letter b_i, $i > 1$. As $(\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi) \mid 1) = (\theta_{\mathcal{Y}}(\phi) \mid 1) = 1$, we deduce

$$\theta(\phi) = \theta_{\mathcal{X}}^{\mathrm{anti}}(\phi)\theta_{\mathcal{Y}}(\phi) = \theta_{\mathcal{X}}^{\mathrm{anti}}(\phi) + \theta_{\mathcal{Y}}(\phi) + \begin{pmatrix}\text{linear combinations of words containing} \\ \text{the letters } b_0 \text{ and } b_i \text{ for some } i > 1\end{pmatrix}.$$

In particular, the part of $\theta(\phi)$ consisting of the letters b_0, b_1 is exactly $\theta_{\mathcal{X}}^{\mathrm{anti}}(\phi)$. Therefore, the injectivity of $\theta_{\mathcal{X}}^{\mathrm{anti}}$ implies the injectivity of θ. □

Since the set $\mathsf{DM}(R)$ is non-empty for any commutative $\mathbb{Q}$-algebra R with unit (Theorem B.25), the existence of the injective map in Theorem 4.21 shows that $\mathsf{BM}(R)$ is non-empty.

Since $\theta : \mathsf{DM} \to \mathsf{BM}$ is an injective natural transformation of affine schemes, we obtain a surjective morphism between the representing algebras (Theorem A.81).

Corollary 4.22. *There is a surjective algebra morphism from $\mathcal{Z}_q^f$ onto the algebra $\mathcal{Z}^f$ of formal multiple zeta values (Definition B.22) given by*

$$\begin{aligned} p: \quad \mathcal{Z}_q^f &\to \mathcal{Z}^f, \\ \zeta_q^f(w) &\mapsto \sum_{\substack{w=uv \\ u\in\mathbb{Q}\langle b_0,b_1\rangle, v\in\mathbb{Q}\langle b_i | i\geq 1\rangle}} \zeta_{⧢}^f\left((\theta_{\mathcal{X}}^{\mathrm{anti}})^{-1}(u)\right)\zeta_*^f\left(\theta_{\mathcal{Y}}^{-1}(v)\right), \qquad (w \in \mathcal{B}^*).\end{aligned}$$

Here $\zeta_*^f(u)$ denotes the stuffle-regularized formal multiple zeta values and $\zeta_{⧢}^f(v)$ denotes the shuffle-regularized formal multiple zeta values (obtained by applying the techniques in Proposition B.5 to the formal multiple zeta values).

Proof. The element $\mathrm{id}_{\mathcal{Z}^f} \in \mathrm{Hom}_{\mathbb{Q}\text{-Alg}}(\mathcal{Z}^f, \mathcal{Z}^f)$ corresponds to the element $\sum_{w\in\mathcal{X}^*} \zeta_{⧢}^f(w)w$ in $\mathsf{DM}(\mathcal{Z}^f)$ under the bijection given in Theorem B.26. We obtain

$$\begin{aligned}\theta\left(\sum_{w\in\mathcal{X}^*}\zeta_{⧢}^f(w)w\right) &= \theta_{\mathcal{X}}^{\mathrm{anti}}\left(\sum_{u\in\mathcal{X}^*}\zeta_{⧢}^f(u)u\right)\theta_{\mathcal{Y}}\left(\sum_{v\in\mathcal{Y}^*}\zeta_*^f(v)v\right) \\ &= \sum_{u\in\mathcal{X}^*,\ v\in\mathcal{Y}^*}\zeta_{⧢}^f(u)\zeta_*^f(v)\theta_{\mathcal{X}}^{\mathrm{anti}}(u)\theta_{\mathcal{Y}}(v) \\ &= \sum_{u\in\{b_0,b_1\}^*,\ v\in\{b_i | i\geq 1\}^*}\zeta_{⧢}^f\Big((\theta_{\mathcal{X}}^{\mathrm{anti}})^{-1}(u)\Big)\zeta_*^f\Big(\theta_{\mathcal{Y}}^{-1}(v)\Big)uv.\end{aligned}$$

So under the bijection given in Theorem 4.18 the element $\theta\Big(\sum_{w\in\mathcal{X}^*}\zeta^f_{ш}(w)w\Big)\in\mathsf{BM}(\mathcal{Z}^f)$ corresponds to the algebra morphism

$$\begin{aligned} p:\quad \mathcal{Z}^f_q &\to \mathcal{Z}^f,\\ \zeta^f_q(w) &\mapsto \sum_{\substack{uv=w\\ u\in\mathbb{Q}\langle b_0,b_1\rangle,\ v\in\mathbb{Q}\langle b_i\mid i\geq 1\rangle}} \zeta^f_{ш}\left((\theta^{\text{anti}}_{\mathcal{X}})^{-1}(u)\right)\zeta^f_*\left(\theta^{-1}_{\mathcal{Y}}(v)\right) \qquad (w\in\mathcal{B}^*). \end{aligned}$$

By Yoneda's Lemma (Theorem A.81) this is exactly the algebra morphism induced by the natural transformation $\theta:\mathsf{DM}\to\mathsf{BM}$ of affine schemes. ☐

Remark 4.23. (i) The map $p:\mathcal{Z}^f_q\to\mathcal{Z}^f$ can be seen as a formal limit $q\to 1$, for example, one computes

$$p(\zeta^f_q(b_2b_3))=\zeta^f_{ш}(\mathbf{1})\zeta^f_*(y_2y_3)=\zeta^f(2,3)$$

and similarly

$$\lim_{q\to 1}(1-q)^5\zeta_q(2,3)=\zeta(2,3).$$

In [BI22, Theorem 4.18] it is proven in a slightly different context that these similarities hold in general. Moreover, in [BIM] a quotient of the algebra of formal multiple Eisenstein series is considered, which is isomorphic to the algebra $\mathcal{Z}^f$ of formal multiple zeta values. The corresponding projection map is similar to the map p.

(ii) In [BKM21] the formal double Eisenstein space $\mathcal{E}_w$ of weight w is introduced and there is a canonical projection $\mathcal{E}_w\to\mathrm{Fil}^{(2)}_D(\mathcal{Z}^f_q)^{(w)}$ (which is on the level of generating series given by $\#^{-1}_Y$, cf. Theorem 2.75). On p. 6 they give a split exact sequence relating the space $\mathcal{E}_w$ to the formal double zeta space $\mathcal{D}_w$ defined for multiple zeta values ([GKZ06]),

$$0\longrightarrow\ker(\pi_w)\longrightarrow\mathcal{E}_w\underset{\sigma_w}{\overset{\pi_w}{\rightleftarrows}}\mathcal{D}_w\longrightarrow 0.$$

If we exclude the case $w=2$, then we have a canonical projection $\mathcal{D}_w\to\mathrm{Fil}^{(2)}_D(\mathcal{Z}^f)^{(w)}$. In particular, the map π_w has some similarities to the projection p.
Moreover, they obtained in Proposition 3.7 a realization in the algebra of quasi-modular forms $\mathcal{E}_k\twoheadrightarrow\widetilde{\mathcal{M}}^{\mathbb{Q}}_k(\mathrm{SL}_2(\mathbb{Z}))$, which might give rise to a non-trivial element in the set $\mathsf{BM}\Big(\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))\Big)$.

4.4 Definition of the space $\mathfrak{bm}_0$

Linearizing the defining equations of the sets $\mathsf{BM}(R)$ (Definition 4.17) yields the definition of the following spaces.

Definition 4.24. For each commutative $\mathbb{Q}$-algebra R with unit, let $\mathfrak{bm}(R)$ be the R-vector space consisting of all non-commutative polynomials $\Psi \in R\langle\mathcal{B}\rangle$ satisfying

$$\begin{array}{llcl} \text{(i)} & (\Psi|b_0) & = & 0, \\ \text{(ii)} & \Delta_q(\Psi) & = & \Psi\otimes\mathbf{1}+\mathbf{1}\otimes\Psi, \\ \text{(iii)} & \tau(\Pi_0(\Psi)) & = & \Pi_0(\Psi). \end{array}$$

Here Π_0 denotes the R-linear extension of the canonical projection $\mathbb{Q}\langle\mathcal{B}\rangle \to \mathbb{Q}\langle\mathcal{B}\rangle^0$ (cf Definition 4.17).

Let $\mathfrak{bm}_0(R)$ be the subspace consisting of all $\Psi \in \mathfrak{bm}(R)$ additionally satisfying

$$\text{(iv)} \quad (\Psi|b_2) = (\Psi|b_4) = (\Psi|b_6) = 0.$$

Denote $\mathfrak{bm} = \mathfrak{bm}(\mathbb{Q})$ and $\mathfrak{bm}_0 = \mathfrak{bm}_0(\mathbb{Q})$ and observe that we have

$$\mathfrak{bm}(R) = \mathfrak{bm}\otimes R, \qquad \mathfrak{bm}_0(R) = \mathfrak{bm}_0\otimes R.$$

Proposition 4.25. *For an element $\Psi \in \mathfrak{bm}(R)$, the condition* (iv) *is equivalent to*

$$(\Psi|b_k b_0^m) = 0, \qquad k \geq 1,\ m\geq 0,\ k+m \text{ even}.$$

Proof. Consider the R-linear map

$$\rho_{\mathcal{B}} : R\langle\mathcal{B}\rangle^0 \to R[X_1, Y_1, X_2, Y_1, \ldots],$$
$$b_{k_1} b_0^{m_0} \ldots b_{k_d} b_0^{m_d} \mapsto X_1^{k_1-1} Y_1^{m_1} \ldots X_d^{k_d-1} Y_d^{m_d}$$

and define for each $f \in R\langle\mathcal{B}\rangle$ the polynomials $\rho_{\mathcal{B}}(f)_0 = 0$ and

$$\rho_{\mathcal{B}}(f)_d\begin{pmatrix} X_1,\ldots,X_d \\ Y_1,\ldots,Y_d\end{pmatrix} = \rho_{\mathcal{B}}\Big(\Pi_0(f)^{(d)}\Big), \quad d\geq 1,$$

where $\Pi_0(f)^{(d)}$ denotes the homogeneous component of $\Pi_0(f)$ of depth d. In the following, we will usually drop the depth index and just write $\rho_{\mathcal{B}}(f)\binom{X_1,\ldots,X_d}{Y_1,\ldots,Y_d}$. Moreover, set

$$\rho_{\mathcal{B}}(f)^{\#_Y}\begin{pmatrix} X_1,\ldots,X_d \\ Y_1,\ldots,Y_d\end{pmatrix} = \rho_{\mathcal{B}}(f)\begin{pmatrix} X_1, X_2, \ldots, X_d \\ Y_1, Y_1+Y_2, \ldots, Y_1+\cdots+Y_d\end{pmatrix}.$$

Then as observed in Theorem 5.46 and Corollary 5.51, for each $\Psi \in \mathfrak{bm}(R)$ the bimould $(\rho_{\mathcal{B}}(\Psi)_d^{\#_Y})_{d\geq 0}$ is alternil and swap invariant. Thus, we have (cf Example C.14 and (C.15.1) considered modulo products)

$$\begin{aligned} 0 &= \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2\end{pmatrix} + \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_2, X_1 \\ Y_2, Y_1\end{pmatrix} + \mathcal{R}_X\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2\end{pmatrix} \\ &= \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1+X_2, X_1 \\ Y_2, Y_1-Y_2\end{pmatrix} + \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1+X_2, X_2 \\ Y_1, Y_2-Y_1\end{pmatrix} + \mathcal{R}_Y\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2\end{pmatrix}, \end{aligned}$$

where

$$\mathcal{R}_X\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} = \frac{\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1 \\ Y_1+Y_2 \end{pmatrix} - \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_2 \\ Y_1+Y_2 \end{pmatrix}}{X_1 - X_2},$$

$$\mathcal{R}_Y\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} = \frac{\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1+X_2 \\ Y_1 \end{pmatrix} - \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1+X_2 \\ Y_2 \end{pmatrix}}{Y_1 - Y_2}.$$

The following computations are similar to [BKM21, Lemma 4.2., Theorem 4.4]. First, we obtain from the above equations

$$\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_2, X_1 \\ Y_2, Y_1 \end{pmatrix} = -\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} - \mathcal{R}_X\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix},$$

$$\begin{aligned}\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1, X_1-X_2 \\ Y_1+Y_2, -Y_2 \end{pmatrix} &= \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1+X_2, X_1 \\ Y_2, Y_1-Y_2 \end{pmatrix}\Big|_{\substack{X_1=X_1-X_2,\ X_2=X_2 \\ Y_1=Y_1,\ Y_2=Y_1+Y_2}} \\ &= -\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} - \mathcal{R}_Y\begin{pmatrix} X_1-X_2, X_2 \\ Y_1, Y_1+Y_2 \end{pmatrix}.\end{aligned}$$

We deduce

$$\begin{aligned}\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_2, X_2-X_1 \\ Y_1+Y_2, -Y_1 \end{pmatrix} &= \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1, X_1-X_2 \\ Y_1+Y_2, -Y_2 \end{pmatrix}\Big|_{\substack{X_1=X_2,\ X_2=X_1 \\ Y_1=Y_2,\ Y_2=Y_1}} \\ &= -\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_2, X_1 \\ Y_2, Y_1 \end{pmatrix} - \mathcal{R}_Y\begin{pmatrix} X_2-X_1, X_1 \\ Y_2, Y_1+Y_2 \end{pmatrix} \\ &= \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} + \mathcal{R}_X\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} - \mathcal{R}_Y\begin{pmatrix} X_2-X_1, X_1 \\ Y_2, Y_1+Y_2 \end{pmatrix}.\end{aligned} \tag{4.25.1}$$

Applying again the same substitution $X_1 = X_2,\ X_2 = X_2 - X_1,\ Y_1 = Y_1 + Y_2,\ Y_2 = -Y_1$ to both sides and then using (4.25.1) leads to

$$\begin{aligned}\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_2-X_1, -X_1 \\ Y_2, -Y_1-Y_2 \end{pmatrix} &= \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_2, X_2-X_1 \\ Y_1+Y_2, -Y_1 \end{pmatrix} + \mathcal{R}_X\begin{pmatrix} X_2, X_2-X_1 \\ Y_1+Y_2, -Y_1 \end{pmatrix} \\ &\quad - \mathcal{R}_Y\begin{pmatrix} -X_1, X_2 \\ -Y_1, Y_2 \end{pmatrix} \\ &= \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} + \mathcal{R}_X\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} - \mathcal{R}_Y\begin{pmatrix} X_2-X_1, X_1 \\ Y_2, Y_1+Y_2 \end{pmatrix} \\ &\quad + \mathcal{R}_X\begin{pmatrix} X_2, X_2-X_1 \\ Y_1+Y_2, -Y_1 \end{pmatrix} - \mathcal{R}_Y\begin{pmatrix} -X_1, X_2 \\ -Y_1, Y_2 \end{pmatrix}.\end{aligned}$$

Finally, applying the same substitution a third time and then using (4.25.1), we end up with

$$\begin{aligned}&\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} -X_1, -X_2 \\ -Y_1, -Y_2 \end{pmatrix} \\ &= \rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_2, X_2-X_1 \\ Y_1+Y_2, -Y_1 \end{pmatrix} + \mathcal{R}_X\begin{pmatrix} X_2, X_2-X_1 \\ Y_1+Y_2, -Y_1 \end{pmatrix} - \mathcal{R}_Y\begin{pmatrix} -X_1, X_2 \\ -Y_1, Y_2 \end{pmatrix}\end{aligned} \tag{4.25.2}$$

$$
\begin{aligned}
&+\mathcal{R}_X\begin{pmatrix} X_2-X_1,-X_1\\ Y_2,-Y_1-Y_2\end{pmatrix}-\mathcal{R}_Y\begin{pmatrix} -X_2,X_2-X_1\\ -Y_1-Y_2,-Y_1\end{pmatrix}\\
=\ &\rho_{\mathcal{B}}(\Psi)^{\#_Y}\begin{pmatrix} X_1,X_2\\ Y_1,Y_2\end{pmatrix}+\mathcal{R}_X\begin{pmatrix} X_1,X_2\\ Y_1,Y_2\end{pmatrix}-\mathcal{R}_Y\begin{pmatrix} X_2-X_1,X_1\\ Y_2,Y_1+Y_2\end{pmatrix}+\mathcal{R}_X\begin{pmatrix} X_2,X_2-X_1\\ Y_1+Y_2,-Y_1\end{pmatrix}\\
&-\mathcal{R}_Y\begin{pmatrix} -X_1,X_2\\ -Y_1,Y_2\end{pmatrix}+\mathcal{R}_X\begin{pmatrix} X_2-X_1,-X_1\\ Y_2,-Y_1-Y_2\end{pmatrix}-\mathcal{R}_Y\begin{pmatrix} -X_2,X_2-X_1\\ -Y_1-Y_2,-Y_1\end{pmatrix}.
\end{aligned}
$$

Observe that we have

$$
\begin{aligned}
\mathcal{R}_X\begin{pmatrix} X_1,X_2\\ Y_1,Y_2\end{pmatrix}&=\sum_{\substack{k_1,k_2\geq 1\\ m_1,m_2\geq 0}}\binom{m_1+m_2}{m_1}(\Psi\mid b_{k_1+k_2}b_0^{m_1+m_2})X_1^{k_1-1}X_2^{k_2-1}Y_1^{m_1}Y_2^{m_2},\\
\mathcal{R}_Y\begin{pmatrix} X_1,X_2\\ Y_1,Y_2\end{pmatrix}&=\sum_{\substack{k_1,k_2\geq 1\\ m_1,m_2\geq 0}}\binom{k_1+k_2-2}{k_1-1}(\Psi\mid b_{k_1+k_2-1}b_0^{m_1+m_2+1})X_1^{k_1-1}X_2^{k_2-1}Y_1^{m_1}Y_2^{m_2}.
\end{aligned}
$$

Thus for $k_1,k_2\geq 1,\ m_1,m_2\geq 0,\ k=k_1+k_2,\ m=m_1+m_2$ and $k+m$ even, the coefficient of $X_1^{k_1-1}X_2^{k_2-1}Y_1^{m_1}Y_2^{m_2}$ in (4.25.2) is given by

$$
\begin{aligned}
0=\ &\binom{m}{m_1}(\Psi\mid b_kb_0^m)-\delta_{k_1,1}\sum_{j=0}^{m}\binom{m-j}{m_1}(\Psi\mid b_{k-1}b_0^{m+1})\\
&+\delta_{m_1,0}(-1)^{k_1-1}\sum_{j=1}^{k-1}\binom{k-j-1}{k_1-1}(\Psi\mid b_kb_0^m)-(-1)^{m_1+k_1-1}\binom{k-2}{k_1-1}(\Psi\mid b_{k-1}b_0^{m+1})\\
&+\delta_{m_2,0}(-1)^{m_1+k_1-1}\sum_{j=1}^{k-1}\binom{k-j-1}{k_1-j}(\Psi\mid b_kb_0^m)-\delta_{k_2,1}\sum_{j=0}^{m}\binom{m-j}{m_2}(\Psi\mid b_{k-1}b_0^{m+1})
\end{aligned}
$$

Note that the terms of depth 2 cancel out, since they only differ by the sign $(-1)^{k-2+m}$. Simplifying the formula, we obtain

$$
\begin{aligned}
&\left(\binom{m}{m_1}+\delta_{m_1,0}(-1)^{k_1-1}\binom{k-1}{k_2-1}+\delta_{m_2,0}(-1)^{m_1+k_1-1}\binom{k-1}{k_2}\right)(\Psi\mid b_kb_0^m)=\\
&\left((-1)^{m_1+k_1-1}\binom{k-2}{k_1-1}+\delta_{k_1,1}\binom{m+1}{m_2}+\delta_{k_2,1}\binom{m+1}{m_2+1}\right)(\Psi\mid b_{k-1}b_0^{m+1})
\end{aligned}\tag{4.25.3}
$$

Assume that $k\geq 6$ and in (4.25.3) choose the case $(k_1,k_2,m_1,m_2)=(k-2,2,0,0)$ and multiply with $\frac{k-3}{2}$ and then subtract the case $(k_1,k_2,m_1,m_2)=(k-3,3,0,0)$ to obtain

$$
\frac{(k+1)(k-1)(k-6)}{12}(\Psi\mid b_kb_0^m)=0.
$$

Therefore, we get for $k>6$ even and $\Psi\in\mathfrak{bm}(R)$ that

$$
(\Psi\mid b_k)=0
$$

and by iteratively applying the identity (4.25.3) we obtain

$$
0=(\Psi\mid b_k)=(\Psi\mid b_{k-1}b_0)=(\Psi\mid b_{k-2}b_0^2)=\cdots=(\Psi\mid b_1b_0^m).
$$

Thus we are left with showing that we can deduce from $(\Psi\mid b_2)=(\Psi\mid b_4)=(\Psi\mid b_6)=0$ that $(\Psi\mid b_kb_0^m)=0$ for $k+m\leq 6$ even. But this follows again from applying iteratively the identity (4.25.3). The converse implication trivially holds. □

In analogy to the case of multiple zeta values (Theorem B.30, Corollary B.31), there is the following big main conjecture.

Conjecture 4.26.

(i) *The space* $\mathfrak{bm}_0$ *admits a weight-graded Lie algebra structure.*

(ii) *The functor* BM_0 *is a pro-unipotent affine group scheme with Lie algebra functor*

$$\widehat{\mathfrak{bm}_0} : \mathbb{Q}\text{-Alg} \to \text{Lie-Alg}, \ R \mapsto \widehat{\mathfrak{bm}_0}(R).$$

(iii) *For any commutative* $\mathbb{Q}$*-algebra* R *with unit and all* $\lambda_1, \lambda_2, \lambda_3 \in R$*, the group* $\mathsf{BM}_0(R)$ *acts freely and transitively on* $\mathsf{BM}_{(\lambda_1,\lambda_2,\lambda_3)}(R)$*. We obtain an isomorphism of affine schemes*

$$\mathbb{A}^3 \times \widehat{\mathfrak{bm}_0} \xrightarrow{\sim} \mathsf{BM},$$

where $\mathbb{A}^3$ *is the affine scheme introduced in Example A.87 for* $V = \mathbb{Q}^3$*.*

Here $\widehat{\mathfrak{bm}_0}(R)$ denotes the completion of $\mathfrak{bm}_0(R)$ with respect to the weight (cf Proposition A.45). As in the case of formal multiple zeta values (Corollary B.32), the following holds.

Theorem 4.27. *Assuming Conjecture 4.26, we obtain an algebra isomorphism*

$$\mathcal{Z}_q^f \simeq \widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z})) \otimes \mathcal{U}(\mathfrak{bm}_0)^\vee.$$

In particular, by Proposition A.35, $\mathcal{Z}_q^f$ *would be a free polynomial algebra.*

Proof. By Proposition A.90 the affine scheme $\widehat{\mathfrak{bm}_0}$ is represented by $\mathcal{S}(\mathfrak{bm}_0^\vee)$, by Theorem 4.18 the affine scheme BM is represented by $\mathcal{Z}_q^f$, and by Example A.87 the affine scheme $\mathbb{A}^3$ is represented by $\mathcal{S}((\mathbb{Q}^3)^*) \simeq \mathbb{Q}[Z_1, Z_2, Z_3]$. So applying Yoneda's Lemma (Theorem A.81) to the isomorphism $\mathbb{A}^3 \times \widehat{\mathfrak{bm}_0} \to \mathsf{BM}$ of affine schemes given in Conjecture 4.26 yields an isomorphism of algebras

$$\mathbb{Q}[Z_1, Z_2, Z_3] \otimes \mathcal{S}(\mathfrak{bm}_0^\vee) \simeq \mathcal{Z}_q^f.$$

By Proposition A.35 we have an algebra isomorphism $\mathcal{S}(\mathfrak{bm}_0^\vee) \simeq \mathcal{U}(\mathfrak{bm}_0)^\vee$ and from classical results in the theory of quasi-modular forms ([MR05, Propositíton 124]) we get $\mathbb{Q}[Z_1, Z_2, Z_3] \simeq \widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$. Thus, we obtain the claimed isomorphy. $\square$

We end the subsection by showing that the double shuffle Lie algebra $\mathfrak{dm}_0$ (Definition B.27) related to multiple zeta values embeds into the space $\mathfrak{bm}_0$.

Theorem 4.28. *There is an embedding of vector spaces*

$$\begin{aligned} \theta : \mathfrak{dm}_0 &\to \mathfrak{bm}_0, \\ \psi &\mapsto \theta_{\mathcal{X}}^{\text{anti}}(\psi) + \theta_{\mathcal{Y}}(\psi_*), \end{aligned}$$

where we denote (as in Definition B.27)

$$\psi_* = \Pi_{\mathcal{Y}}(\psi) + \psi_{\text{corr}} = \Pi_{\mathcal{Y}}(\psi) + \sum_{n \geq 2} \frac{(-1)^{n-1}}{n} (\Pi_{\mathcal{Y}}(\psi) | y_n) y_1^n$$

and the maps $\theta_{\mathcal{X}}^{\text{anti}}$, $\theta_{\mathcal{Y}}$ *are defined in* (4.19.1), (4.7.2).

Proof. Let $\psi \in \mathfrak{dm}_0$. Then one has $(\psi \mid x_0) = 0$ and hence $(\theta(\psi) \mid b_0) = 0$. Since the maps $\theta_{\mathcal{X}}^{\mathrm{anti}}$ and $\theta_{\mathcal{Y}}$ are coalgebra morphisms and the elements $\psi,\ \psi_*$ are primitive for $\Delta_{\sqcup\!\sqcup},\ \Delta_*$, one obtains

$$\begin{aligned}\Delta_q(\theta(\psi)) &= \Delta_q\Big(\theta_{\mathcal{X}}^{\mathrm{anti}}(\psi) + \theta_{\mathcal{Y}}(\psi_*)\Big) = \mathbf{1} \otimes \theta_{\mathcal{X}}^{\mathrm{anti}}(\psi) + \theta_{\mathcal{X}}^{\mathrm{anti}}(\psi) \otimes \mathbf{1} + \mathbf{1} \otimes \theta_{\mathcal{Y}}(\psi_*) + \theta_{\mathcal{Y}}(\psi_*) \otimes \mathbf{1} \\ &= \mathbf{1} \otimes \theta(\psi) + \theta(\psi) \otimes \mathbf{1}.\end{aligned}$$

By definition of the map $\theta_{\mathcal{Y}}$, the image $\theta_{\mathcal{Y}}(\psi_*)$ does not contain the letter b_0, and thus $\Pi_0(\theta_{\mathcal{Y}}(\psi_*)) = \theta_{\mathcal{Y}}(\psi_*)$. Together with Lemma 4.20, compute

$$\begin{aligned}\tau\Big(\Pi_0(\theta(\psi))\Big) &= \tau\Big(\Pi_0(\theta_{\mathcal{X}}^{\mathrm{anti}}(\psi))\Big) + \tau\Big(\theta_{\mathcal{Y}}(\psi_*)\Big) \\ &= \theta_{\mathcal{Y}}\Big(\Pi_{\mathcal{Y}}(\psi)\Big) + \tau\Big(\theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi))\Big) + \tau\Big(\theta_{\mathcal{Y}}(\psi_{\mathrm{corr}})\Big) \\ &= \theta_{\mathcal{Y}}\Big(\Pi_{\mathcal{Y}}(\psi)\Big) + \Pi_0\Big(\theta_{\mathcal{X}}^{\mathrm{anti}}(\psi)\Big) + \theta_{\mathcal{Y}}(\psi_{\mathrm{corr}}) \\ &= \Pi_0\Big(\theta_{\mathcal{X}}^{\mathrm{anti}}(\psi)\Big) + \theta_{\mathcal{Y}}(\psi_*) \\ &= \Pi_0\Big(\theta(\psi)\Big).\end{aligned}$$

For the third equality observe that $\theta_{\mathcal{Y}}(\psi_{\mathrm{corr}})$ consists of the letter b_1 and is therefore τ-invariant. Finally, we obtain from Proposition B.29 that $(\psi \mid x_0^{k-1}x_1) = 0$ for $k \geq 2$ even and thus $(\theta(\psi) \mid b_2) = (\theta(\psi) \mid b_4) = (\theta(\psi) \mid b_6) = 0$. Altogether, the element $\theta(\psi)$ is contained in $\mathfrak{bm}_0$ and thus the map θ is well-defined. Since $\theta_{\mathcal{X}}^{\mathrm{anti}}$ and $\theta_{\mathcal{Y}}$ are injective, also the map θ is injective. □

4.5 Calculating the space $\mathfrak{bm}_0$

We will present an algorithm to compute a basis for $\mathfrak{bm}_0$ in some given weight w. The computations are partly similar to the ones done in [ENR03] for multiple zeta values. In particular, implementing the algorithm allows us to compute the dimensions of the homogeneous subspaces $\mathfrak{bm}_0^{(w)}$ for weight $w \leq 13$ and observe that they coincide with the dimension conjecture 1.22 (iii). The computations will be done in a new alphabet $\mathcal{V}$.

Definition 4.29. For each $k \geq 1$, denote by v_k the homogeneous part of weight k of $\log\Big(\mathbf{1} + \sum_{l\geq 1} b_l\Big)$, this means

$$v_k = \sum_{\substack{l_1+\dots+l_d=k \\ l_1,\dots,l_d\geq 1}} \frac{(-1)^{d+1}}{d} b_{l_1}\dots b_{l_d}.$$

Moreover set $v_0 = b_0$ and let $\mathcal{V}$ be the alphabet consisting of the letters v_i, $i \geq 0$. We define the weight and depth for a word in $\mathbb{Q}\langle\mathcal{V}\rangle$ as

$$\mathrm{wt}(v_{s_1}\dots v_{s_l}) = s_1 + \dots + s_l + |\{i \mid s_i = 0\}|, \qquad \mathrm{dep}(v_{s_1}\dots v_{s_l}) = l - |\{i \mid s_i = 0\}|.$$

Example 4.30. One computes

$$\begin{aligned}
v_1 &= b_1, \\
v_2 &= b_2 - \frac{1}{2}b_1^2, \\
v_3 &= b_3 - \frac{1}{2}b_1b_2 - \frac{1}{2}b_2b_1 + \frac{1}{3}b_1^3, \\
v_4 &= b_4 - \frac{1}{2}b_1b_3 - \frac{1}{2}b_2b_2 - \frac{1}{2}b_3b_1 + \frac{1}{3}b_1^2b_2 + \frac{1}{3}b_1b_2b_1 + \frac{1}{3}b_2b_1^2 - \frac{1}{4}b_1^4.
\end{aligned}$$

Lemma 4.31. *The alphabet $\mathcal{V}$ generates the algebra* $(\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc})$.

Proof. For all $k \geq 1$, one has

$$b_k = \sum_{\substack{l_1+\dots+l_d=k \\ l_1,\dots,l_d\geq 1}} \frac{1}{d!} v_{l_1}\dots v_{l_d}. \tag{4.31.1}$$

Since the letters $b_0 = v_0$ and b_k, $k \geq 1$, are the canonical algebra generators of $\mathbb{Q}\langle\mathcal{B}\rangle$, we obtain the claim. □

Observe that the notions of weight and depth defined for the alphabet $\mathcal{V}$ (Definition 4.29) and the alphabet $\mathcal{B}$ (Definition 2.11) induce the same filtrations on the algebra $\mathbb{Q}\langle\mathcal{B}\rangle$.

Proposition 4.32. *The primitive elements of* $(\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc}, \Delta_q)$ *are exactly given by* $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$.

Proof. Let $\mathcal{A} = \{a_0, a_1, a_2, \dots\}$ be a countable alphabet and equip the free non-commutative algebra $(\mathbb{Q}\langle\mathcal{A}\rangle, \mathrm{conc})$ with the shuffle coproduct (Example A.62)

$$\Delta_{ш}(a_i) = a_i \otimes \mathbf{1} + \mathbf{1} \otimes a_i, \qquad i \geq 0,$$

so $\Delta_{ш}$ is compatible with the concatenation product. We show that we have a Hopf algebra isomorphism

$$\begin{aligned}
\sigma : (\mathbb{Q}\langle\mathcal{A}\rangle, \mathrm{conc}, \Delta_{ш}) &\xrightarrow{\sim} (\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc}, \Delta_q), \\
a_i &\mapsto v_i.
\end{aligned}$$

Since the primitive elements of $\mathbb{Q}\langle\mathcal{A}\rangle$ are exactly given by $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{A}\rangle$ (Corollary A.40), we deduce $\mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle) = \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$. Clearly, σ is an algebra isomorphism, thus we only have to check that σ is a coalgebra morphism. We obtain

$$\begin{aligned}\Delta_q\left(\mathbf{1}+\sum_{l\geq 1} b_l\right) &= \mathbf{1}\otimes\mathbf{1}+\sum_{l\geq 1}\Big(\mathbf{1}\otimes b_l + b_l\otimes\mathbf{1}+\sum_{\substack{l_1+l_2=l\\ l_1,l_2\geq 1}} b_{l_1}\otimes b_{l_2}\Big)\\ &= \left(\mathbf{1}+\sum_{l\geq 1} b_l\right)\otimes\left(\mathbf{1}+\sum_{l\geq 1} b_l\right),\end{aligned}$$

so the element $\mathbf{1}+\sum_{l\geq 1} b_l$ is grouplike for the coproduct Δ_q. Therefore, Theorem A.51 implies that $\log\Big(\mathbf{1}+\sum_{l\geq 1} b_l\Big)$ is primitive for Δ_q. Since the coproduct Δ_q is graded for the weight, also the homogeneous components v_k, $k\geq 1$, of $\log\Big(\mathbf{1}+\sum_{l\geq 1} b_l\Big)$ are primitive. Moreover, the element $v_0 = b_0$ is by definition primitive for Δ_q. We deduce for each $i \geq 0$

$$\Delta_q(\sigma(a_i)) = \Delta_q(v_i) = \mathbf{1}\otimes v_i + v_i\otimes\mathbf{1} = \mathbf{1}\otimes\sigma(a_i)+\sigma(a_i)\otimes\mathbf{1} = (\sigma\otimes\sigma)(\Delta_{\sqcup\!\sqcup}(a_i)).$$

Hence σ is a coalgebra morphism. □

Since one requirement on the elements in $\mathfrak{bm}_0$ is to be primitive for the coproduct Δ_q, we obtain the following.

Corollary 4.33. *We have an inclusion* $\mathfrak{bm}_0 \subset \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$.

In particular, the first step towards a basis of some homogeneous space $\mathfrak{bm}_0^{(w)}$ is to compute a basis for the homogeneous space $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle^{(w)}$ in some weight w. More precisely, we will compute the Lyndon basis (Definition A.12, Theorem A.13). We start by generating a list of all Lyndon words in the alphabet $\mathcal{V}$ up to some weight w.

Proposition 4.34. *([BP94, chapter 2]) The following variant of Duval's algorithm computes for some given Lyndon word $w \in \mathbb{Q}\langle\mathcal{V}\rangle$ of weight $\leq n$ the next Lyndon word of weight $\leq n$.*

Algorithm 1 *Duval's algorithm*

- *Input: Lyndon word $w \in \mathbb{Q}\langle\mathcal{V}\rangle$, weight $n\in\mathbb{N}$*
- *Generate the word u of length n, whose ith letter is equal to the ith letter of w modulo the length of w*
- *While $\mathrm{wt}(u) > n$ omit the last letter of u*
- *If $\mathrm{wt}(u) = n$ and the last letter of u is not equal to v_0, omit the last letter of u*
- *Replace the last letter v_i of u by v_{i+1}*
- *Output: u*

□

In particular, starting with the smallest Lyndon word v_0 in the alphabet $\mathcal{V}$ and successively applying Duval's algorithm to the previous output yields a list of all Lyndon words in $\mathcal{V}$ of weight $\leq n$. The procedure stops at the Lyndon word v_n, since the next output of Duval's algorithm is the empty word.

Example 4.35. Up to weight 5, one obtains successively the following Lyndon words by applying Duval's algorithm (Proposition 4.34)

$v_0,\quad v_0v_0v_0v_0v_1,\quad v_0v_0v_0v_1,\quad v_0v_0v_0v_1v_1,\quad v_0v_0v_0v_2,\quad v_0v_0v_1,\quad v_0v_0v_1v_0v_1,\quad v_0v_0v_1v_1,$
$v_0v_0v_1v_1v_1,\quad v_0v_0v_1v_2,\quad v_0v_0v_2,\quad v_0v_0v_2v_1,\quad v_0v_0v_3,\quad v_0v_1,\quad v_0v_1v_0v_1v_1,\quad v_0v_1v_0v_2,$
$v_0v_1v_1,\quad v_0v_1v_1v_1,\quad v_0v_1v_1v_1v_1,\quad v_0v_1v_1v_2,\quad v_0v_1v_2,\quad v_0v_1v_2v_1,\quad v_0v_1v_3,\quad v_0v_2,$
$v_0v_2v_1,\quad v_0v_2v_1v_1,\quad v_0v_2v_2,\quad v_0v_3,\quad v_0v_3v_1,\quad v_0v_4,\quad v_1,\quad v_1v_1v_1v_2,\quad v_1v_1v_2,\quad v_1v_1v_3,$
$v_1v_2,\quad v_1v_2v_2,\quad v_1v_3,\quad v_1v_4,\quad v_2,\quad v_2v_3,\quad v_3,\quad v_4,\quad v_5.$

Next, we compute the standard bracket of each Lyndon word (Definition A.12 (ii)).

Proposition 4.36. *([Lo05, p. 15]) For an arbitrary word $w \in \mathbb{Q}\langle\mathcal{V}\rangle$, the following algorithm computes the length (first output) and the multiplicity (second output) of the first Lyndon factor of w.*

***Algorithm 2** Lyndon factorization*

- `Input:` `Word` $w \in \mathbb{Q}\langle\mathcal{V}\rangle$
- `Set` $i = 0$, $j = 1$
- `While` j `is smaller than the length of` w `and the` $(i+1)$`-th letter of` w `is smaller or equal to the` $(j+1)$`-th letter of` w`, do:`
  - `If the` $(i+1)$`-th letter is smaller than the` $(j+1)$`-th letter of` w`, set` $i = 0$`; else increase` i `by` 1
  - `Increase` j `by` 1
- `Output:` $\left(j-i, \left\lfloor \frac{j}{j-i} \right\rfloor\right)$

□

Consider some Lyndon word $w \in \mathbb{Q}\langle\mathcal{V}\rangle$ and write $w = v_i\widetilde{w}$ with $v_i \in \mathcal{V}$ and $\widetilde{w} \in \mathbb{Q}\langle\mathcal{V}\rangle$. Successively applying the previous algorithm to the word $\widetilde{w}$ yields the Lyndon factorization

$$\widetilde{w} = l_1^{n_1} \dots l_r^{n_r}, \quad l_1 > \dots > l_r \text{ Lyndon words.}$$

Then the word l_r is the longest suffix of $\widetilde{w}$ and hence the longest nontrivial suffix of w, which is a Lyndon word ([Re93, Lemma 7.14]). Thus, the standard bracket of w (Definition A.12) is recursively given by

$$\gamma(w) = [\gamma(v_i l_1^{n_1} \dots l_{r-1}^{n_{r-1}} l_r^{n_r - 1}), \gamma(l_r)].$$

From Theorem A.13, one directly obtains the following.

Proposition 4.37. *The standard brackets $\gamma(w)$, $w \in \mathbb{Q}\langle\mathcal{V}\rangle$ Lyndon word, give a basis for the space* $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$*.*

Example 4.38. By applying the algorithm in Proposition 4.36, one obtains successively the following basis for the homogeneous subspaces of $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$ up to weight 5:

$v_0,\quad v_1,\quad v_2,\quad ,v_3,\quad ,v_4,\quad v_5,\quad [v_0,v_1],\quad [v_0,v_2],\quad [v_0,v_3],\quad [v_0,v_4],\quad [v_1,v_2],$
$[v_1,v_3],\quad [v_1,v_4],\quad [v_2,v_3],\quad [v_0,[v_0,v_1]],\quad [v_0,[v_0,v_2]],\quad [v_0,[v_0,v_3]],\quad [[v_0,v_1],v_1],$
$[v_0,[v_1,v_2]],\quad [v_0,[v_1,v_3]],\quad [[v_0,v_2],v_1],\quad [[v_0,v_2],v_2],\quad [[v_0,v_3],v_1],\quad [v_1,[v_1,v_2]],$
$[v_1,[v_1,v_3]],\quad [[v_1,v_2],v_2],\quad [v_0,[v_0,[v_0,v_1]]],\quad [v_0,[v_0,[v_0,v_2]]],\quad [v_0,[[v_0,v_1],v_1]],$
$[v_0,[v_0,[v_1,v_2]]],\quad [v_0,[[v_0,v_2],v_1]],\quad [[v_0,v_1],[v_0,v_2]],\quad [[[v_0,v_1],v_1],v_1],$
$[v_0,[v_1,[v_1,v_2]]],\quad [[v_0,[v_1,v_2]],v_1],\quad [[[v_0,v_2],v_1],v_1],\quad [v_1,[v_1,[v_1,v_2]]],$
$[v_0,[v_0,[v_0,[v_0,v_1]]]],\quad [v_0,[v_0,[[v_0,v_1],v_1]]],\quad [[v_0,[v_0,v_1]],[v_0,v_1]],$
$[v_0,[[[v_0,v_1],v_1],v_1]],\quad [[v_0,v_1],[[v_0,v_1],v_1]],\quad [[[[v_0,v_1],v_1],v_1],v_1].$

The last step for computing a basis of $\mathfrak{bm}_0^{(w)}$ is to determine the subspace in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle^{(w)}$ spanned by the elements, whose projections to $\mathbb{Q}\langle\mathcal{B}\rangle^0$ are τ-invariant.

Theorem 4.39. *Let $n > 1$ be given. Then the following steps lead to a basis for the homogeneous subspace $\mathfrak{bm}^{(n)}$ of weight n:*

1) Compute the standard brackets $\gamma(w)$ for all Lyndon words $w \in \mathbb{Q}\langle\mathcal{V}\rangle$ of weight n (Proposition 4.34, 4.36).

2) Rewrite all standard brackets $\gamma(w)$ from step 1) in the alphabet $\mathcal{B}$ (Definition 4.29) and apply the projection Π_0.

3) Compute a basis for the intersection of $\ker(\tau - \mathrm{id})$ and the vector space spanned by the elements obtained in step 2).

4) In the basis obtained in step 3) replace all the projections with their original standard brackets.

If $n = 2, 4, 6$ omit the elements containing the word v_n to obtain a basis of $\mathfrak{bm}_0^{(n)}$. In all other cases, one has $\mathfrak{bm}_0^{(n)} = \mathfrak{bm}^{(n)}$.

Unfortunately, the size of the matrices in step 3) increases very fast, hence we were able to execute the algorithm only up to weight 13.

Example 4.40. 1) Without any algorithm it is easy to see that the homogeneous subspace $\mathfrak{bm}_0^{(1)}$ is spanned by the element

$$\xi\begin{pmatrix}1\\0\end{pmatrix} = v_1.$$

2) To determine a basis for $\mathfrak{bm}_0^{(2)}$, we first compute the projections of the standard brackets of weight 2 (obtained in Example 4.38):

$$\sigma_1^{(2)} = b_2 - \frac{1}{2}b_1b_1, \qquad \sigma_2^{(2)} = -b_1b_0.$$

Restricting the map $\tau - \mathrm{id}$ to $\mathrm{span}_{\mathbb{Q}}\{\sigma_1^{(2)}, \sigma_2^{(2)}\}$ we obtain that the kernel is spanned by

$$\sigma_1^{(2)} - \sigma_2^{(2)}.$$

Thus the space $\mathfrak{bm}^{(2)}$ is spanned by the element $v_2 - [v_0, v_1]$ and the space $\mathfrak{bm}_0$ is empty.

3) In weight 3, we have the following projections of the standard brackets (given in Example 4.38)

$$\sigma_1^{(3)} = b_3 - \frac{1}{2}b_1b_2 - \frac{1}{2}b_2b_1 + \frac{1}{3}b_1b_1b_1, \quad \sigma_2^{(3)} = -b_2b_0 + \frac{1}{2}b_1b_1b_0, \quad \sigma_3^{(3)} = b_1b_2 - b_2b_1,$$
$$\sigma_4^{(3)} = b_1b_0b_0, \quad \sigma_5^{(3)} = -2b_1b_0b_1 + b_1b_1b_0.$$

The kernel of the map $\tau - \mathrm{id}$ restricted to $\mathrm{span}_{\mathbb{Q}}\{\sigma_1^{(3)}, \sigma_2^{(3)}, \sigma_3^{(3)}, \sigma_4^{(3)}, \sigma_5^{(3)}\}$ has the basis

$$\sigma_1^{(3)} - \frac{3}{2}\sigma_3^{(3)} + \sigma_4^{(3)} + \sigma_5^{(3)}, \qquad -\sigma_2^{(3)} + \sigma_3^{(3)} - \frac{1}{2}\sigma_5^{(3)}.$$

Thus a basis for the homogeneous subspace $\mathfrak{bm}_0^{(3)}$ is given by

$$\xi\begin{pmatrix}3\\0\end{pmatrix} = v_3 - \frac{3}{2}[v_1, v_2] + [v_0, [v_0, v_1]] + [[v_0, v_1], v_1],$$
$$\xi\begin{pmatrix}2\\1\end{pmatrix} = -[v_0, v_2] + [v_1, v_2] - \frac{1}{2}[[v_0, v_1], v_1].$$

4) A basis for $\mathfrak{bm}^{(4)}$ is given by

$$\xi\begin{pmatrix}2,1\\1,0\end{pmatrix} = [[v_0, v_2], v_1] + 2[v_0, [v_1, v_2]] - [v_1, [v_1, v_2]] + \frac{1}{2}[[[v_0, v_1], v_1], v_1],$$
$$v_4 - \frac{5}{2}[v_0, v_3] + \frac{5}{2}[v_0, [v_0, v_2]] - [v_0, [v_0, [v_0, v_1]]] + \frac{1}{2}[v_1, v_3] - \frac{5}{4}[v_0, [v_1, v_2]]$$
$$- \frac{1}{4}[v_0, [[v_0, v_1], v_1]] + \frac{5}{12}[v_1, [v_1, v_2]] - \frac{1}{6}[[[v_0, v_1], v_1], v_1].$$

In particular, the first element spans the space $\mathfrak{bm}_0^{(4)}$.

5) A basis for $\mathfrak{bm}_0^{(5)}$ is given by the elements

$$\begin{aligned}
\xi\begin{pmatrix}5\\0\end{pmatrix} = \; & v_5 + [v_0, [v_0, [v_0, [v_0, v_1]]]] - \frac{5}{2}[v_1, v_4] + 5[v_2, v_3] + 2[v_0, [v_0, [[v_0, v_1], v_1]]] \\
& - \frac{3}{2}[[v_0, [v_0, v_1]], [v_0, v_1]] + \frac{5}{12}[v_1, [v_1, v_3]] - \frac{25}{12}[[v_1, v_2], v_2] + 2[v_0, [[[v_0, v_1], v_1], v_1]] \\
& + \frac{1}{2}[[v_0, v_1], [[v_0, v_1], v_1]] - \frac{5}{4}[v_1, [v_1, [v_1, v_2]]] + [[[[v_0, v_1], v_1], v_1], v_1], \\
\xi\begin{pmatrix}4\\1\end{pmatrix} = \; & - [v_0, v_4] - [v_0, [v_0, [v_0, v_2]]] + [v_1, v_4] - \frac{3}{2}[v_2, v_3] - \frac{1}{2}[v_0, [v_1, v_3]] - 2[[v_0, v_3], v_1] \\
& + \frac{3}{2}[[v_0, v_2], v_2] - \frac{1}{2}[v_0, [v_0, [[v_0, v_1], v_1]]] + \frac{1}{2}[[v_0, [v_0, v_1]], [v_0, v_1]] + [v_0, [v_0, [v_1, v_2]]] \\
& - [v_0, [[v_0, v_2], v_1]] - 2[[v_0, v_1], [v_0, v_2]] - \frac{3}{4}[v_1, [v_1, v_3]] - \frac{3}{4}[[v_1, v_2], v_2] \\
& + \frac{11}{6}[v_0, [v_1, [v_1, v_2]]] + 3[[v_0, [v_1, v_2]], v_1] + \frac{1}{6}[[[v_0, v_2], v_1], v_1] - \frac{1}{2}[v_0, [[[v_0, v_1], v_1], v_1]] \\
& - \frac{1}{2}[[v_0, v_1], [[v_0, v_1], v_1]] - \frac{1}{8}[v_1, [v_1, [v_1, v_2]]] + \frac{1}{8}[[[[v_0, v_1], v_1], v_1], v_1], \\
\xi\begin{pmatrix}3\\2\end{pmatrix} = \; & [v_0, [v_0, v_3]] + \frac{3}{2}[[v_0, v_3], v_1] - [[v_0, v_2], v_2] - \frac{1}{2}[v_0, [v_0, [v_1, v_2]]] + \frac{1}{2}[v_0, [[v_0, v_2], v_1]] \\
& + \frac{3}{2}[[v_0, v_1], [v_0, v_2]] + \frac{1}{2}[v_1, [v_1, v_3]] + [[v_1, v_2], v_2] - [v_0, [v_1, [v_1, v_2]]] \\
& - \frac{7}{4}[[v_0, [v_1, v_2]], v_1] - \frac{1}{12}[v_0, [[[v_0, v_1], v_1], v_1]] + \frac{1}{4}[[v_0, v_1], [[v_0, v_1], v_1]] \\
& + \frac{1}{4}[v_1, [v_1, [v_1, v_2]]] - \frac{1}{4}[[[[v_0, v_1], v_1], v_1], v_1], \\
\xi\begin{pmatrix}2,1,1\\1,0,0\end{pmatrix} = \; & -3[v_0, [v_1, [v_1, v_2]]] - 3[[v_0, [v_1, v_2]], v_1] - [[[v_0, v_2], v_1], v_1] + [v_1, [v_1, [v_1, v_2]]] \\
& - \frac{1}{2}[[[[v_0, v_1], v_1], v_1], v_1].
\end{aligned}$$

Recall that we expect the following dimensions for the homogeneous subspaces of the universal enveloping algebra of $\mathfrak{bm}_0$ (Conjecture 1.22 (iii))

$$H_{\mathcal{U}(\mathfrak{bm}_0)}(x) = \sum_{w\geq 0} \dim_{\mathbb{Q}} \mathcal{U}(\mathfrak{bm}_0)^{(w)} x^w \overset{?}{=} \frac{1}{1 - D(x)O_1(x) + D(x)R(x)}.$$

Lemma 4.41. *There are integers $g_w \in \mathbb{Z}$, such that*

$$\frac{1}{1 - D(x)O_1(x) + D(x)R(x)} = \prod_{w\geq 1} (1 - x^w)^{-g_w}.$$

Proof. This is a simple application of [Bou89, p. 140, Lemma 1]. □

If $(1 - D(x)O_1(X) + D(x)R(x))^{-1}$ is indeed the Hilbert-Poincare series of the universal enveloping algebra $\mathcal{U}(\mathfrak{bm}_0)$, then by Proposition A.35 and Corollary A.7 we must have $g_w \geq 0$ for all $w \geq 1$. In particular, Conjecture 1.22 (iii) is equivalent to the following.

Conjecture 4.42. *For all $w \geq 1$, we have*

$$\dim_{\mathbb{Q}} \mathfrak{bm}_0^{(w)} = g_w.$$

For example, for $w \leq 14$ the following values are obtained in [BK20]:

w	1	2	3	4	5	6	7	8	9	10	11	12	13	14
g_w	1	0	2	1	4	3	8	11	18	28	48	74	126	202

We continued the calculations illustrated in Example 4.40 to obtain the following.

Theorem 4.43. *For each $w \leq 13$, we have*

$$\dim_{\mathbb{Q}} \mathfrak{bm}_0^{(w)} = g_w.$$

Proof. Execution of the algorithm given in Theorem 4.39 with the computer algebra system PARI/GP. □

The algorithm solves linear equations in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$. Since

$$\begin{aligned}\sum_{w\geq 0} \dim_{\mathbb{Q}} \mathcal{U}(\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle)^{(w)} x^w &= \frac{1}{1 - 2x - x^2 - x^3 - x^4 - x^5 - \dots} \\ &= 1 + 2x + 5x^2 + 13x^3 + 34x^4 + 89x^5 + 233x^6 + 610x^7 \\ &\quad + 1597x^8 + 4181x^9 + 10946x^{10} + 28657x^{11} + 75025x^{12} \\ &\quad + 196418x^{13} + 514229x^{14} + \dots,\end{aligned}$$

sophisticated methods are needed to verify Conjecture 4.42 for higher weights.

4.6 Alternative description of $\mathfrak{bm}_0$ in the alphabet $\mathcal{C}^{\text{bi}}$

For further studies of the space $\mathfrak{bm}_0$, we will introduce a third alphabet. In this new alphabet, the elements in $\mathfrak{bm}_0$ possess the shortest representation. In should be seen as a q-analog of the alphabet $\mathcal{C}$ defined for multiple zeta values (Definition B.65).

Definition 4.44. For $k \geq 1,\ m \geq 0$, define

$$C_{k,m} = \Big(-\operatorname{ad}(v_0)\Big)^m (v_k) = [\dots[[v_k, \underbrace{v_0], v_0], \dots, v_0]}_{m \text{ times}}$$

and denote by $\mathcal{C}^{\text{bi}}$ the alphabet consisting of all these letters.

Proposition 4.45. *(Lazard elimination, [Re93, Theorem 0.6]) The space* $\operatorname{Lie}_{\mathbb{Q}}\langle \mathcal{C}^{\text{bi}}\rangle$ *is a free Lie algebra and*

$$\operatorname{Lie}_{\mathbb{Q}}\langle \mathcal{V}\rangle = \mathbb{Q}v_0 \oplus \operatorname{Lie}_{\mathbb{Q}}\langle \mathcal{C}^{\text{bi}}\rangle. \qquad \square$$

By considering the universal enveloping algebras and applying Lemma 4.31, one obtains

$$\mathbb{Q}\langle \mathcal{B}\rangle = \mathbb{Q}[v_0] \otimes \mathbb{Q}\langle \mathcal{C}^{\text{bi}}\rangle. \tag{4.45.1}$$

In the following, we will always make use of the fact that the alphabet $\mathcal{V}$ provides a free generating set for the algebra $(\mathbb{Q}\langle \mathcal{B}\rangle, \text{conc})$ (Lemma 4.31).

Definition 4.46. Let $\partial_0 : \mathbb{Q}\langle \mathcal{B}\rangle \to \mathbb{Q}\langle \mathcal{B}\rangle$ be the derivation with respect to concatenation given by $\partial_0(v_0) = 1$ and $\partial_0(v_k) = 0$ for all $k \geq 1$.

Proposition 4.47. *(i) The kernel of the derivation* ∂_0 *is exactly given by* $\mathbb{Q}\langle \mathcal{C}^{\text{bi}}\rangle$*.*
(ii) The restriction of $\Pi_0 : \mathbb{Q}\langle \mathcal{B}\rangle \to \mathbb{Q}\langle \mathcal{B}\rangle^0$ *to* $\ker(\partial_0)$ *has an inverse given by*

$$\begin{aligned} \sec_q : \mathbb{Q}\langle \mathcal{B}\rangle^0 &\to \mathbb{Q}\langle \mathcal{B}\rangle, \\ f &\mapsto \sum_{m\geq 0} \frac{(-1)^m}{m!} v_0^m \partial_0^m(f). \end{aligned}$$

In particular, the image of $\sec_q$ is contained in $\ker(\partial_0)$.

Proof. (i) Follows directly from the decomposition in (4.45.1).
(ii) For any $f \in \mathbb{Q}\langle \mathcal{B}\rangle^0$, compute

$$\begin{aligned} \partial_0\Big(\sec_q(f)\Big) &= \sum_{m\geq 0} \frac{(-1)^m}{m!} \partial_0\Big(v_0^m \partial_0^m(f)\Big) \\ &= \sum_{m\geq 1} \frac{(-1)^m}{(m-1)!} v_0^{m-1} \partial_0^m(f) + \sum_{m\geq 0} \frac{(-1)^m}{m!} v_0^m \partial_0^{m+1}(f) \\ &= 0. \end{aligned}$$

We deduce $\operatorname{im}(\sec_q) \subset \ker(\partial_0)$. Since $\Pi_0(v_0^m \partial_0(f)) = 0$ for all $m \geq 1$, we obtain for $f \in \mathbb{Q}\langle \mathcal{B}\rangle^0$

$$\Pi_0\Big(\sec_q(f)\Big) = \Pi_0(f) = f.$$

So Π_0 has the right inverse $\sec_q$. Next, let $g \in \ker(\partial_0)$ and write $g = \sum_{m\geq 0} v_0^m g_m$ with $g_m \in \mathbb{Q}\langle \mathcal{B}\rangle^0$. Then compute

$$0 = \partial_0(g) = \sum_{m\geq 1} m v_0^{m-1} g_m + \sum_{m\geq 0} v_0^m \partial_0(g_m)$$

Since $g_m \in \mathbb{Q}\langle\mathcal{B}\rangle^0$ for all $m \geq 0$, one obtains $\partial_0(g_m) \in \mathbb{Q}\langle\mathcal{B}\rangle^0$. Thus coefficient comparison with respect to v_0 at the beginning leads to

$$0 = mg_m + \partial_0(g_{m-1}), \qquad m \geq 1.$$

Inductively, we deduce for all $m \geq 1$

$$g_m = \frac{(-1)^m}{m!}\partial_0^m(g_0)$$

and thus get

$$\mathrm{sec}_q\Big(\Pi_0(g)\Big) = \mathrm{sec}_q(g_0) = \sum_{m\geq 0}\frac{(-1)^m}{m!}v_0^m\partial_0^m(g_0) = \sum_{m\geq 0} v_0^m g_m = g.$$

So sec_q is also the left inverse for the restriction of Π_0 to $\ker(\partial_0)$. □

The map sec_q allows extending the involution τ (see (4.8.2)) to the algebra $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$.

Definition 4.48. Define the map $\tau_{\mathcal{C}^{\mathrm{bi}}} : \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle \to \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$ to be the composition

$$\tau_{\mathcal{C}^{\mathrm{bi}}} = \mathrm{sec}_q \circ \tau \circ \Pi_0.$$

Explicitly, the map $\tau_{\mathcal{C}^{\mathrm{bi}}}$ can be computed as follows:

1) Translate words in $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$ into words in $\mathbb{Q}\langle\mathcal{B}\rangle$ (Definition 4.29, 4.44).
2) Apply the map $\tau \circ \Pi_0$.
3) Translate words in $\mathbb{Q}\langle\mathcal{B}\rangle$ into words in $\mathbb{Q}\langle\mathcal{V}\rangle$ (see (4.31.1)).
4) Translate words in $\mathbb{Q}\langle\mathcal{V}\rangle$ into words in $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$ by using iteratively the identity

$$\begin{aligned}&\mathrm{sec}_q(C_{k_1,m_1}\cdots C_{k_j,m_j}v_0C_{k_{j+1},m_{j+1}}\cdots C_{k_d,m_d})\\ &\qquad = \sum_{i=1}^{j} C_{k_1,m_1}\dots C_{k_{i-1},m_{i-1}}C_{k_i,m_i+1}C_{k_{i+1},m_{i+1}}\dots C_{k_d,m_d}.\end{aligned}$$

In particular, the letter v_0 acts like a right derivation on $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$.

Example 4.49. We compute

$$\begin{aligned}\tau_{\mathcal{C}^{\mathrm{bi}}}(C_{2,1}) &= \mathrm{sec}_q \circ\tau\circ\Pi_0\left((b_2-\frac{1}{2}b_1^2)b_0 - b_0(b_2-\frac{1}{2}b_1^2)\right)\\ &= \mathrm{sec}_q\left(b_2b_0 - \frac{1}{2}b_2b_1\right)\\ &= \mathrm{sec}_q\left(v_2v_0 + \frac{1}{2}v_1^2v_0 - \frac{1}{2}v_2v_1 - \frac{1}{4}v_1^3\right)\\ &= \mathrm{sec}_q\left(C_{2,0}v_0 + \frac{1}{2}C_{1,0}^2v_0 - \frac{1}{2}C_{2,0}C_{1,0} - \frac{1}{4}C_{1,0}^3\right)\\ &= C_{2,1} + \frac{1}{2}C_{1,1}C_{1,0} + \frac{1}{2}C_{1,0}C_{1,1} - \frac{1}{2}C_{2,0}C_{1,0} - \frac{1}{4}C_{1,0}^3\end{aligned}$$

Definition 4.50. We define the following subspaces of $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$

$$\begin{aligned}\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle^{\tau} &= \left\{f\in\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle \;\middle|\; \tau_{\mathcal{C}^{\mathrm{bi}}}(f) = f\right\},\\ \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle^{\tau}_{-} &= \left\{f\in\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle^{\tau} \;\middle|\; (f\mid C_{2,0}) = (f\mid C_{4,0}) = (f\mid C_{6,0}) = 0\right\}.\end{aligned}$$

The spaces $\mathfrak{bm}$ and $\mathfrak{bm}_0$ can be purely described in terms of the alphabet $\mathcal{C}^{\mathrm{bi}}$.

Theorem 4.51. *The following holds*

$$\mathfrak{bm} \simeq \mathrm{Lie}_{\mathbb{Q}}\langle \mathcal{C}^{\mathrm{bi}} \rangle \cap \mathbb{Q}\langle \mathcal{C}^{\mathrm{bi}} \rangle^{\tau}, \qquad \mathfrak{bm}_0 \simeq \mathrm{Lie}_{\mathbb{Q}}\langle \mathcal{C}^{\mathrm{bi}} \rangle \cap \mathbb{Q}\langle \mathcal{C}^{\mathrm{bi}} \rangle^{\underline{\tau}}.$$

Proof. By Proposition 4.32, the primitive elements of $(\mathbb{Q}\langle \mathcal{B} \rangle, \mathrm{conc}, \Delta_q)$ are exactly given by $\mathrm{Lie}_{\mathbb{Q}}\langle \mathcal{V} \rangle$. Applying additionally the Lazard elimination (Proposition 4.45), one obtains that $\Psi \in \mathbb{Q}\langle \mathcal{B} \rangle$ satisfies $(\Psi \mid b_0) = 0$ and $\Delta_q(\Psi) = \Psi \otimes 1 + 1 \otimes \Psi$ if and only if $\Psi \in \mathrm{Lie}_{\mathbb{Q}}\langle \mathcal{C}^{\mathrm{bi}} \rangle$. Furthermore, by the construction of the map $\tau_{\mathcal{C}^{\mathrm{bi}}}$, Ψ satisfies $\tau(\Pi_0(\Psi)) = \Pi_0(\Psi)$ if and only if $\Psi \in \mathbb{Q}\langle \mathcal{C}^{\mathrm{bi}} \rangle^{\tau}$. So by definition of the space $\mathfrak{bm}$ (Definition 4.24), we obtain then $\mathfrak{bm} \simeq \mathrm{Lie}_{\mathbb{Q}}\langle \mathcal{C}^{\mathrm{bi}} \rangle \cap \mathbb{Q}\langle \mathcal{C}^{\mathrm{bi}} \rangle^{\tau}$.
For each $k \geq 1$, $C_{k,0}$ is the unique word in $\mathbb{Q}\langle \mathcal{C}^{\mathrm{bi}} \rangle$, which contains the word b_k (when rewritten in the alphabet $\mathcal{B}$ according to Definition 4.44, 4.29). Thus, $\Psi \in \mathbb{Q}\langle \mathcal{B} \rangle$ satisfies $(\Psi \mid b_k) = 0$ for $k = 2, 4, 6$ if and only if $(\Psi \mid C_{k,0}) = 0$ for $k = 2, 4, 6$. This shows the second isomorphism. □

4.7 The structure of $\mathfrak{bm}_0$

We will explain the conjectured Lie algebra structure of $\mathfrak{bm}_0$. In particular, we will describe the expected generators and relations in $\mathfrak{bm}_0$ and present a systematic list in small weights.

Let $(\mathfrak{mq}, \{-,-\}_q)$ be the q-twisted Magnus Lie algebra (Theorem 3.20), where $\{-,-\}_q$ denotes the q-Ihara bracket. Then as a refinement of Conjecture 4.26 (i), we expect the following.

Conjecture 4.52. *The space* $\mathfrak{bm}_0$ *is a weight-graded Lie subalgebra of* $(\mathfrak{mq}, \{-,-\}_q)$.

Example 4.53. As obtained in Example 4.40, the following two elements are contained in $\mathfrak{bm}_0$

$$\xi\binom{1}{0} = b_1, \qquad \xi\binom{2}{1} = b_2b_0 - b_0b_2 + b_1b_2 - b_2b_1 - b_1^2b_0 + b_1b_0b_1.$$

We compute

$$\begin{aligned}\left\{\xi\binom{2}{1}, \xi\binom{1}{0}\right\}_q = & -b_1b_0b_2 + 2b_0b_1b_2 + 2b_2b_1b_0 - b_2b_0b_1 - b_1b_2b_0 - b_0b_2b_1 + 2b_1^2b_0b_1 \\ & - b_1b_0b_1^2 - b_1^3b_0 - b_1^2b_2 + 2b_1b_2b_1 - b_2b_1^2 \\ & \in \mathfrak{bm}_0.\end{aligned}$$

The elements in $\mathfrak{bm}_0$ as well as the formula for the q-Ihara bracket $\{-,-\}_q$ are quite complicated, but it is checked with computer assistance that Conjecture 4.52 holds up to weight 9. Moreover, the space $\mathfrak{bm}_0$ is isomorphic to the space $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ of bimoulds (Corollary 5.51), which is also expected to be a Lie algebra (Conjecture 5.19). The q-Ihara bracket and the conjectural Lie bracket on $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ are compatible with this isomorphism (Theorem 5.52). Finally, the associated depth-graded space to $\mathfrak{bm}_0$ embeds into a Lie algebra $(\mathfrak{lq}, \{-,-\}_q^D)$ (Theorem 4.63), where $\{-,-\}_q^D$ is exactly the depth-graded Lie bracket to the q-Ihara bracket $\{-,-\}_q$.

If one could show that the q-Ihara bracket $\{-,-\}_q$ preserves the primitive elements of $(\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc}, \Delta_q)$ and τ-invariance, this would give a proof for Conjecture 4.52. Since the primitive elements of $(\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc}, \Delta_q)$ are exactly the elements in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$, the invariance of the primitive elements under $\{-,-\}_q$ should follow from a closed formula for the q-Ihara bracket or the derivation d_w^q (Definition 3.12) in terms of the alphabet $\mathcal{V}$.

Example 4.54. With some computer assistance, one computes the following.

(i) For all $w \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$, we have $d_w^q(v_0) = 0$

(ii) For all $w \in \mathrm{Lie}_{\mathbb{Q}}\langle v_0, v_1\rangle$ and $i \geq 0$, we have $d_w^q(v_i) = [w, v_i]$

(iii) For all $i \geq 1$, we have $d_{v_2}^q(v_i) = [v_2, v_i] - [v_1, v_i]$

(iv) We have

$$\begin{aligned}d^q_{[v_0,v_2]}(v_1) &= [[v_0, v_2], v_1] - [[v_0, v_1], v_2] + \frac{1}{2}[[v_1, [v_0, v_1]], v_1],\\ d^q_{[v_0,v_2]}(v_2) &= [[v_0, v_2], v_2] - [[v_0, v_1], v_3] + \frac{1}{2}[[v_1, [v_0, v_1]], v_2] + \frac{1}{12}[[v_1, [v_1, [v_0, v_1]]], v_1]\\ d^q_{[v_0,v_2]}(v_3) &= [[v_0, v_2], v_3] - [[v_0, v_1], v_4] + \frac{1}{2}[[v_1, [v_0, v_1]], v_3] + \frac{1}{12}[[v_1, [v_1, [v_0, v_1]]], v_2]\\ &\quad + \frac{1}{12}[v_1, [[v_1, [v_0, v_1]], v_2]]\end{aligned}$$

$$
\begin{aligned}
d^q_{[v_0,v_2]}(v_4) &= [[v_0,v_2],v_4] - [[v_0,v_1],v_5] + \frac{1}{2}[[v_1,[v_0,v_1]],v_4] + \frac{1}{12}[[v_1,[v_1,[v_0,v_1]]],v_3]\\
&+ \frac{1}{12}[v_1,[[v_1,[v_0,v_1]],v_3]] + \frac{1}{12}[[v_2,[v_1,[v_0,v_1]]],v_2]\\
&- \frac{1}{720}[[v_1,[v_1,[v_1,[v_1,[v_0,v_1]]]]],v_1]
\end{aligned}
$$

(v) We have

$$
\begin{aligned}
d^q_{v_3}(v_1) &= [v_3,v_1] - 2[v_2,v_2] + [v_1,v_3] + \frac{3}{2}[[v_1,v_2],v_1]\\
d^q_{v_3}(v_2) &= [v_3,v_2] - 2[v_2,v_3] + [v_1,v_4] + \frac{3}{2}[[v_1,v_2],v_2] + \frac{1}{4}[[v_1,[v_1,v_2]],v_1]\\
d^q_{v_3}(v_3) &= [v_3,v_3] - 2[v_2,v_4] + [v_1,v_5] + \frac{3}{2}[[v_1,v_2],v_3] + \frac{1}{4}[[v_1,[v_1,v_2]],v_2]\\
&+ \frac{1}{4}[v_1,[[v_1,v_2],v_2]]\\
d^q_{v_3}(v_4) &= [v_3,v_4] - 2[v_2,v_5] + [v_1,v_6] + \frac{3}{2}[[v_1,v_2],v_4] + \frac{1}{4}[[v_1,[v_1,v_2]],v_3]\\
&+ \frac{1}{4}[v_1,[[v_1,v_2],v_3]] + \frac{1}{4}[[v_2,[v_1,v_2]],v_2] - \frac{1}{240}[[v_1,[v_1,[v_1,[v_1,v_2]]]],v_1]\\
d^q_{v_3}(v_5) &= [v_3,v_5] - 2[v_2,v_6] + [v_1,v_7] + \frac{3}{2}[[v_1,v_2],v_5] + \frac{1}{4}[[v_1,[v_1,v_2]],v_4]\\
&+ \frac{1}{4}[v_1,[[v_1,v_2],v_4]] + \frac{1}{4}[[v_2,[v_1,v_2]],v_3] + \frac{1}{4}[v_2,[[v_1,v_2],v_3]]\\
&- \frac{1}{240}[[v_1,[v_1,[v_1,[v_1,v_2]]]],v_2] - \frac{1}{240}[v_1,[v_1,[v_1,[[v_1,v_2],v_2]]]]\\
&- \frac{1}{240}[v_1,[v_1,[[v_1,[v_1,v_2]],v_2]]] - \frac{1}{240}[v_1,[[v_1,[v_1,[v_1,v_2]]],v_2]]
\end{aligned}
$$

All values of the derivation d^q_w in the previous example are contained in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$, which means primitive elements of $(\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc}, \Delta_q)$ get mapped to primitive elements in these special cases. It is not clear how to find such a general formula for the derivation d^q_w on $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$, which allows deducing the invariance of the primitive elements under this derivation.

Furthermore, one easily checks that the q-Ihara bracket does not preserve τ-invariance in general, this holds only true for τ-invariant primitive elements in $(\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc}, \Delta_q)$. But it is not clear, how to prove this property of the q-Ihara bracket $\{-,-\}_q$ in general.

Finally, we want to give an insight into the expected structure of $(\mathfrak{bm}_0, \{-,-\}_q)$ as shortly stated in Conjecture 1.22. At the end of this subsection, we will systematically present the generators and relations of $\mathfrak{bm}_0$ in low weights.

We expect that $\mathfrak{bm}_0$ has besides the generator $\xi\binom{1}{0} = b_1$ one generator $\xi\binom{k}{0}$ in each odd weight $k \geq 3$, which lies in the image of the embedding $\theta : \mathfrak{dm}_0 \to \mathfrak{bm}_0$ (Theorem 4.28). Moreover, there should be a derivation on $\mathfrak{bm}_0$, which increases the weight by 2. We denote the m-th derivative of the element $\xi\binom{k}{0}$ by $\xi\binom{k+m}{m}$. Conjecturally, the elements $\xi\binom{k}{m}$, $k \geq 1$, $m \geq 0$, $k+m$ odd, provide a complete generating set for the Lie algebra $(\mathfrak{bm}_0, \{-,-\}_q)$. In particular, denote $D(x) = \frac{1}{1-x^2}$ and $O_1(x) = \frac{x}{1-x^2}$, then the coefficient of $D(x)O_1(x)$ at x^w would be equal to the number of generators of $\mathfrak{bm}_0$ in weight w.

Remark 4.55. Since an element in $\mathfrak{bm}_0$ must be contained in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$ and τ-invariant on

$\mathbb{Q}\langle\mathcal{B}\rangle^0$, the depth-graded part $\mathrm{gr}_D\,\xi\binom{k}{m}$ of the generator $\xi\binom{k}{m}$ must be given by

$$\mathrm{gr}_D\,\xi\begin{pmatrix}k\\m\end{pmatrix} = \Big(-\operatorname{ad}(b_0)\Big)^m(b_k) + \Big(-\operatorname{ad}(b_0)\Big)^{k-1}(b_{m+1}).$$

These elements should provide a complete set of generators for the associated depth-graded Lie algebra to $\mathfrak{bm}_0$ in depth 1.

In contrast to the case of the double shuffle Lie algebra $\mathfrak{dm}_0$ related to multiple zeta values (Conjecture B.33), we do not expect that $\mathfrak{bm}_0$ is a free Lie algebra. More precisely, we conjecture that the generators of $\mathfrak{bm}_0$ described above satisfy exactly $\dim(\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))) + \dim(\mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z})))$ independent relations in weight k and also derivatives of these relations. The relations between the generators of $\mathfrak{bm}_0$ corresponding to the Eisenstein series are given by the following.

Proposition 4.56. *If* $(\mathfrak{bm}_0, \{-,-\}_q)$ *is a Lie algebra (Conjecture 4.52), then we have for all* $k \geq 1$ *odd*

$$\left\{\xi\begin{pmatrix}k\\0\end{pmatrix}, \xi\begin{pmatrix}1\\0\end{pmatrix}\right\}_q = 0.$$

Proof. For $k = 1$ the equation holds trivially, thus we assume $k \geq 3$. Then by definition, the element $\xi\binom{k}{0}$ is an element in the image of the embedding $\theta: \mathfrak{dm}_0 \to \mathfrak{bm}_0$ (Theorem 4.28). Let $w \in \mathbb{Q}\langle\mathcal{B}\rangle$ be a word, such that the coefficient of w in $\xi\binom{k}{0}$ is nonzero. Then due to the construction of the map θ, this means that w consists of the letters b_0, b_1 or does not contain the letter b_0. In the first case, we obtain from Lemma 3.15 (i) that

$$\left\{w, \xi\begin{pmatrix}1\\0\end{pmatrix}\right\}_q = d_w^q(b_1) - d_{b_1}^q(w) - [w, b_1] = [w, b_1] - 0 - [w, b_1] = 0.$$

Since the q-Ihara bracket preserves the subspace of $\mathbb{Q}\langle\mathcal{B}\rangle$ spanned by words, which do not contain the letter b_0, we obtain from the previous calculation that $\{\xi\binom{k}{0}, \xi\binom{1}{0}\}$ does not contain the letter b_0. We assumed that $(\mathfrak{bm}_0, \{-,-\}_q)$ is a Lie algebra, so in particular, the element $\{\xi\binom{k}{0}, \xi\binom{1}{0}\}_q$ must be τ-invariant. By definition of the map τ any τ-invariant element, which does not contain the letter b_0, must consist of powers of b_1. Since $\{-,-\}_q$ is homogeneous for the weight (Lemma 3.15 (ii)), we deduce

$$\left\{\xi\begin{pmatrix}k\\0\end{pmatrix}, \xi\begin{pmatrix}1\\0\end{pmatrix}\right\}_q = \lambda b_1^{k+1} \qquad \text{for some } \lambda \in \mathbb{Q}.$$

The bracket $\{\xi\binom{k}{0}, \xi\binom{1}{0}\}_q$ is contained in $\mathfrak{bm}_0$ and hence is an element in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$. Since $b_1^{k+1} \notin \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$, we deduce $\lambda = 0$ and therefore

$$\left\{\xi\begin{pmatrix}k\\0\end{pmatrix}, \xi\begin{pmatrix}1\\0\end{pmatrix}\right\}_q = 0.$$

□

Derivatives of the Eisenstein relations given in Proposition 4.56 should be of the form

$$\sum_{\substack{m_1+m_2=m\\ m_1,m_2\geq 0}} \binom{m}{m_1} \left\{\xi\begin{pmatrix}k+m_1\\m_1\end{pmatrix}, \xi\begin{pmatrix}1+m_2\\m_2\end{pmatrix}\right\}_q = 0, \qquad k \geq 1 \text{ odd}.$$

It is not clear how to describe the relations between the generators of $\mathfrak{bm}_0$ corresponding to the cusp forms $\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ in general.

We expect that the previously explained described structure determines $(\mathfrak{bm}_0, \{-,-\}_q)$ completely. Thus by (A.11.1), the Hilbert-Poincare series of $\mathcal{U}(\mathfrak{bm}_0)$ should be given by

$$H_{\mathcal{U}(\mathfrak{bm}_0)}(x) = \sum_{w\geq 0} \dim_{\mathbb{Q}} \mathcal{U}(\mathfrak{bm}_0)^{(w)} x^w \stackrel{?}{=} \frac{1}{1-D(x)O_1(x)+D(x)R(x)}, \tag{4.56.1}$$

where

$$D(x) = \frac{1}{1-x^2}, \qquad O_1(x) = \frac{x}{1-x^2}, \qquad R(x) = \sum_{k\geq 4} \dim\Big(\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))\oplus\mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z}))\Big)x^k.$$

We expect an algebra isomorphism $\mathcal{Z}_q^f \simeq \mathcal{Z}_q$, thus Theorem 4.27 should also lead to a decomposition

$$\mathcal{Z}_q \simeq \widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z})) \otimes \mathcal{U}(\mathfrak{bm}_0)^\vee.$$

Applying Lemma A.2, one obtains that this decomposition of $\mathcal{Z}_q$ as well as the dimension conjecture (4.56.1) and the dimension conjecture 1.21 for $\mathcal{Z}_q$ are compatible. Even more, the dimension conjectures (4.56.1) and 1.21 should be equivalent.

We want to investigate $\mathfrak{bm}_0$ systematically in small weights. More precisely, we will list the Lie algebra generators in each weight and also linearly independent Lie products. Both together will give a basis for $\mathfrak{bm}_0$ in these weights. Moreover, we will give the non-trivial relations between the Lie algebra generators, which means we will only consider relations not induced by the anti-symmetry or Jacobi's identity for the q-Ihara bracket. The elements will be described in the alphabet $\mathcal{C}^{\mathrm{bi}}$, since this gives the shortest expression.

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weight 1

Generators:

$$\xi\binom{1}{0} = C_{1,0}$$

Relations: ——

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weight 2

Generators: ——

Relations: ——

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weight 3

Generators:

$$\xi\binom{3}{0} = C_{3,0} + C_{1,2} - \frac{3}{2}[C_{1,0}, C_{2,0}] - [C_{1,1}, C_{1,0}]$$

$$\xi\binom{2}{1} = C_{2,1} + [C_{1,0}, C_{2,0}] + \frac{1}{2}[C_{1,1}, C_{1,0}]$$

Relations: ——

---

weight 4

Generators: ———

Lie products:

$$\left\{\xi\binom{2}{1},\xi\binom{1}{0}\right\}_q = [C_{2,1},C_{1,0}] - 2[C_{1,1},C_{2,0}] - [C_{1,0},[C_{1,0},C_{2,0}]] - \frac{1}{2}[[C_{1,1},C_{1,0}],C_{1,0}]$$

Relations:

$$\left\{\xi\binom{3}{0},\xi\binom{1}{0}\right\}_q = 0$$

---

weight 5

Generators:

$$\begin{aligned}\xi\binom{5}{0} &= C_{5,0} + C_{1,4} - \frac{5}{2}[C_{1,0},C_{4,0}] + 5[C_{2,0},C_{3,0}] - 2[C_{1,3},C_{1,0}] - \frac{1}{2}[C_{1,2},C_{1,1}] \\ &\quad + \frac{5}{12}[C_{1,0},[C_{1,0},C_{3,0}]] - \frac{25}{12}[[C_{1,0},C_{2,0}],C_{2,0}] + 2[[C_{1,2},C_{1,0}],C_{1,0}] \\ &\quad - \frac{3}{2}[C_{1,1},[C_{1,1},C_{1,0}]] - \frac{5}{4}[C_{1,0},[C_{1,0},[C_{1,0},C_{2,0}]]] - [[[C_{1,1},C_{1,0}],C_{1,0}],C_{1,0}] \\ \xi\binom{4}{1} &= C_{4,1} + C_{2,3} + [C_{1,0},C_{4,0}] - \frac{3}{2}[C_{2,0},C_{3,0}] + \frac{1}{2}[C_{1,1},C_{3,0}] - \frac{3}{2}[C_{1,0},C_{3,1}] \\ &\quad - \frac{3}{2}[C_{2,1},C_{2,0}] + \frac{1}{2}[C_{1,3},C_{1,0}] + [C_{1,2},C_{2,0}] + [C_{1,1},C_{2,1}] + 2[C_{1,0},C_{2,2}] \\ &\quad - \frac{3}{4}[C_{1,0},[C_{1,0},C_{3,0}]] - \frac{3}{4}[[C_{1,0},C_{2,0}],C_{2,0}] - \frac{11}{6}[C_{1,1},[C_{1,0},C_{2,0}]] \\ &\quad + \frac{7}{6}[C_{1,0},[C_{1,1},C_{2,0}]] + [C_{1,0},[C_{1,0},C_{2,1}]] - \frac{1}{2}[[C_{1,2},C_{1,0}],C_{1,0}] \\ &\quad - \frac{1}{8}[C_{1,0},[C_{1,0},[C_{1,0},C_{2,0}]]] - \frac{1}{8}[[[C_{1,1},C_{1,0}],C_{1,0}],C_{1,0}] \\ \xi\binom{3}{2} &= C_{3,2} - \frac{3}{2}[C_{3,1},C_{1,0}] + [C_{2,1},C_{2,0}] - \frac{1}{2}[C_{1,2},C_{2,0}] - [C_{1,0},C_{2,2}] \\ &\quad + \frac{1}{2}[C_{1,0},[C_{1,0},C_{3,0}]] + [[C_{1,0},C_{2,0}],C_{2,0}] + [C_{1,1},[C_{1,0},C_{2,0}]] \\ &\quad - \frac{3}{4}[C_{1,0},[C_{1,1},C_{2,0}]] - \frac{3}{4}[C_{1,0},[C_{1,0},C_{2,1}]] - \frac{1}{12}[[C_{1,2},C_{1,0}],C_{1,0}] \\ &\quad + \frac{1}{3}[C_{1,1},[C_{1,1},C_{1,0}]] + \frac{1}{4}[C_{1,0},[C_{1,0},[C_{1,0},C_{2,0}]]] + \frac{1}{4}[[[C_{1,1},C_{1,0}],C_{1,0}],C_{1,0}]\end{aligned}$$

Lie products:

$$\begin{aligned}\left\{\left\{\xi\binom{2}{1},\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q &= 3[C_{1,1},[C_{1,0},C_{2,0}]] + [C_{1,0},[C_{1,0},C_{2,1}]] \\ &\quad + [C_{1,0},[C_{1,0},[C_{1,0},C_{2,0}]]] + \frac{1}{2}[[[C_{1,1},C_{1,0}],C_{1,0}],C_{1,0}]\end{aligned}$$

Relations: ———

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weight 6

Generators: ———

Lie products:

$$\left\{\xi\binom{4}{1},\xi\binom{1}{0}\right\}_q, \qquad \left\{\xi\binom{3}{2},\xi\binom{1}{0}\right\}_q, \qquad \left\{\left\{\left\{\xi\binom{2}{1},\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q$$

Relations:

$$\left\{\xi\binom{5}{0},\xi\binom{1}{0}\right\}_q=0, \qquad \left\{\xi\binom{4}{1},\xi\binom{1}{0}\right\}_q+\left\{\xi\binom{3}{0},\xi\binom{2}{1}\right\}_q=0$$

---

weight 7

Generators:

$$\xi\binom{7}{0}, \qquad \xi\binom{6}{1}, \qquad \xi\binom{5}{2}, \qquad \xi\binom{4}{3}$$

Lie products:

$$\left\{\left\{\xi\binom{4}{1},\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q, \qquad \left\{\left\{\xi\binom{3}{2},\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,$$

$$\left\{\xi\binom{2}{1},\left\{\xi\binom{2}{1},\xi\binom{1}{0}\right\}_q\right\}_q, \qquad \left\{\left\{\left\{\left\{\xi\binom{2}{1},\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q$$

Relations: ———

---

weight 8

Generators: ———

Lie products:

$$\left\{\xi\binom{6}{1},\xi\binom{1}{0}\right\}_q, \qquad \left\{\xi\binom{5}{2},\xi\binom{1}{0}\right\}_q, \qquad \left\{\xi\binom{4}{3},\xi\binom{1}{0}\right\}_q, \qquad \left\{\xi\binom{5}{0},\xi\binom{3}{0}\right\}_q,$$

$$\left\{\xi\binom{4}{1},\xi\binom{3}{0}\right\}_q, \qquad \left\{\xi\binom{4}{1},\xi\binom{2}{1}\right\}_q, \qquad \left\{\xi\binom{3}{2},\xi\binom{2}{1}\right\}_q,$$

$$\left\{\left\{\left\{\xi\binom{4}{1},\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q, \qquad \left\{\left\{\left\{\xi\binom{3}{2},\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,$$

$$\left\{\left\{\xi\binom{2}{1},\left\{\xi\binom{2}{1},\xi\binom{1}{0}\right\}_q\right\}_q,\xi\binom{1}{0}\right\}_q,$$

$$\left\{\left\{\left\{\left\{\left\{\xi\binom{2}{1},\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q,\xi\binom{1}{0}\right\}_q$$

Relations:

$$\left\{\xi\binom{7}{0},\xi\binom{1}{0}\right\}_q=0, \qquad \left\{\xi\binom{6}{1},\xi\binom{1}{0}\right\}_q+\left\{\xi\binom{5}{0},\xi\binom{2}{1}\right\}_q=0,$$

$$\left\{\xi\binom{5}{2},\xi\binom{1}{0}\right\}_q+2\left\{\xi\binom{4}{1},\xi\binom{2}{1}\right\}_q+\left\{\xi\binom{3}{0},\xi\binom{3}{2}\right\}_q=0$$

4.8 The depth-graded balanced q-shuffle Lie algebra

We study the defining equations for $\mathfrak{bm}_0$ modulo higher depth. This leads to a q-analog of the linearized double shuffle Lie algebra $\mathfrak{ls}$ (Definition B.36).

Consider the usual shuffle coproduct $\Delta_{ш}$ on $\mathbb{Q}\langle\mathcal{B}\rangle$ (Example A.62), i.e., set

$$\Delta_{ш}(b_i) = b_i \otimes \mathbf{1} + \mathbf{1} \otimes b_i, \quad i \geq 0,$$

and extend this with respect to the concatenation product.

Definition 4.57. Let $\mathfrak{lq}$ be the vector space given by all non-commutative polynomials $\Psi \in \mathbb{Q}\langle\mathcal{B}\rangle$ satisfying

$$\begin{array}{cccc} \text{(i)} & (\Psi|b_0) & = & 0, \\ \text{(ii)} & \Delta_{ш}(\Psi) & = & \Psi \otimes \mathbf{1} + \mathbf{1} \otimes \Psi, \\ \text{(iii)} & \tau(\Pi_0(\Psi)) & = & \Pi_0(\Psi), \\ \text{(iv)} & (\Psi|b_k b_0^m) & = & 0, \qquad k+m \text{ even.} \end{array}$$

By Corollary A.40 condition (ii) is equivalent to $\Psi \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{B}\rangle$.

Definition 4.58. Denote the associated depth-graded space to $\mathfrak{bm}_0$ by

$$\mathfrak{lb} = \mathrm{gr}_D\, \mathfrak{bm}_0.$$

Proposition 4.59. *There is an embedding of vector spaces*

$$\mathfrak{lb} \hookrightarrow \mathfrak{lq}.$$

Proof. Let $\Psi \in \mathfrak{bm}_0$. Then evidently the associated depth-graded element $\mathrm{gr}_D\,\Psi$ also satisfies $(\mathrm{gr}_D\,\Psi \mid b_0) = 0$ and we also have $\tau(\Pi_0(\mathrm{gr}_D\,\Psi)) = \Pi_0(\mathrm{gr}_D\,\Psi)$, since τ is homogeneous in depth. Furthermore, we have $\mathrm{gr}_D\,\Delta_q = \Delta_{ш}$, thus $\mathrm{gr}_D\,\Psi$ is primitive for the coproduct $\Delta_{ш}$. Finally, by Proposition 4.25, we have $(\Psi \mid b_k b_0^m) = 0$ for all $k+m$ even, and therefore the same holds for the associated depth-graded element $\mathrm{gr}_D\,\Psi$. □

In contrast to the case of multiple zeta values, it turns out that the associated depth-graded space $\mathfrak{lb}$ is not isomorphic to $\mathfrak{lq}$.

Example 4.60. The following element of weight 8 and depth 2 is contained in $\mathfrak{lq}$, but not in $\mathfrak{lb}$:

$$b_3b_0b_2b_0b_0 - b_2b_0b_3b_0b_0 + b_2b_0b_0b_3b_0 - b_3b_0b_0b_2b_0 - b_0b_0b_2b_3b_0 + b_0b_0b_3b_2b_0 + b_0b_2b_3b_0b_0$$
$$- b_0b_3b_2b_0b_0 - b_0b_0b_3b_0b_2 + b_0b_0b_2b_0b_3 - b_0b_2b_0b_0b_3 + b_0b_3b_0b_0b_2.$$

Definition 4.61. For a word $w = b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}$ in $\mathbb{Q}\langle\mathcal{B}\rangle$, define the derivation $d_w^{q,D}$ on $(\mathbb{Q}\langle\mathcal{B}\rangle, \cdot)$ by

$$\begin{aligned} d_w^{q,D}(\mathbf{1}) &= d_w^{q,D}(b_0) = 0, \\ d_w^{q,D}(b_a) &= \delta_{d+1}(w b_a) - \delta_1(b_a w_1) \\ &= \sum_{l_1=0}^{k_1-1} \cdots \sum_{l_d=0}^{k_d-1} \binom{k_1-1}{l_1} \cdots \binom{k_d-1}{l_d} (-1)^{l_1+\dots+l_d} \\ &\qquad\qquad \cdot \left[b_0^{m_0} b_{k_1-l_1} b_0^{m_1} \dots b_{k_d-l_d} b_0^{m_d}, b_{i+l_1+\dots+l_d} \right], \end{aligned}$$

where $a \geq 1$.

The operator δ_j is given in Definition 3.8

Definition 4.62. For $f, g \in \mathbb{Q}\langle\mathcal{B}\rangle$, the depth-graded q-Ihara bracket $\{-,-\}_q^D$ is given by

$$\{f,g\}_q^D = d_f^{q,D}(g) - d_g^{q,D}(f) - [f,g].$$

We obtain from the definition of the derivations $d_w^{q,D}$ (Definition 4.61) and d_w^q (Definition 3.12) that $\{-,-\}_q^D$ is exactly the associated depth-graded to the q-Ihara bracket $\{-,-\}_q$ (Definition 3.16).

Theorem 4.63. *The pair* $(\mathfrak{lq}, \{-,-\}_q^D)$ *is a bi-graded Lie algebra.*

Proof. The proof relies on the comparison of the space $\mathfrak{lq}$ and a Lie algebra consisting of bimoulds, thus see Corollary 5.71 □

Since the associated depth-graded space $\mathfrak{lb}$ to $\mathfrak{bm}_0$ is a subspace of $\mathfrak{lq}$ and $\{-,-\}_q^D$ is exactly the associated depth-graded Lie bracket to the q-Ihara bracket $\{-,-\}_q$, Conjecture 4.52 would imply the following.

Conjecture 4.64. *The space* $\mathfrak{lb}$ *is a bi-graded Lie subalgebra of* $(\mathfrak{lq}, \{-,-\}_q^D)$.

Remark 4.65. We expect that $\mathfrak{lb}$ is generated by two Lie sub algebras $\mathfrak{F}$ and $\mathfrak{D}$, where $\mathfrak{F}$ is generated in depth 1 (by the elements given in Remark 4.55) and $\mathfrak{D}$ is generated in depth 4. The generators of the Lie algebra $\mathfrak{F}$ satisfy some relations in depth 2 related to (tensor products of) modular forms and the generators of $\mathfrak{F}$ and $\mathfrak{D}$ satisfy some relations in depth 5. This should determine $\mathfrak{lb}$ completely. We will study this in detail in the commutative approach involving bimoulds (Subsection 5.2).

Next, we equip the Lie algebra $(\mathfrak{lq}, \{-,-\}_q^D)$ with a derivation.

Proposition 4.66. *(Lazard elimination, [Re93, Theorem 0.6]) The Lie algebra* $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{B}\rangle$ *is generated by the elements* b_0 *and*

$$\Big(-\operatorname{ad}(b_0)\Big)^m(b_k) = [\dots[[b_k,b_0],b_0],\dots,b_0], \qquad k \geq 1,\ m \geq 0.$$

Definition 4.67. Define the derivation (with respect to the concatenation product) $\delta : \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{B}\rangle \to \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{B}\rangle$ by

$$\delta\Big(\Big(-\operatorname{ad}(b_0)\Big)^m(b_k)\Big) = \Big(-\operatorname{ad}(b_0)\Big)^{m+1}(b_{k+1}).$$

Note that the derivation δ increases the weight by 2.

Proposition 4.68. *The tuple* $(\mathfrak{lq}, \{-,-\}_q^D, \delta)$ *is a differential Lie algebra.*

Proof. To shorten the notation, set $D_{k,m} = \Big(-\operatorname{ad}(b_0)\Big)^m(b_k)$. Since both maps $\{-,-\}_q^D$ and δ are $\mathbb{Q}$-linear, we can assume $f = D_{k_1,m_1}\dots D_{k_d,m_d}$ and $g = D_{l_1,n_1}\dots D_{l_e,n_e}$. We compute straight-forwardly

$$\delta\Big(d_f^q(g)\Big) = \delta\Bigg(\sum_{i=1}^{e}\sum_{k_1'=0}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\binom{k_1-1}{k_1'}\cdots\binom{k_d-1}{k_d'}(-1)^{k_1+\dots+k_d'}$$
$$\cdot D_{l_1,n_1}\dots D_{l_{i-1},n_{i-1}}\Big(-\operatorname{ad}(b_0)\Big)^{n_i}\Big(\Big[D_{k_1-k_1',m_1}\dots D_{k_d-k_d',m_d}, D_{l_i+k_1'+\dots+k_d',0}\Big]\Big)$$
$$\cdot D_{l_{i+1},n_{i+1}}\dots D_{l_e,n_e}\Bigg)$$

$$
\begin{aligned}
&= \sum_{i=1}^{e}\sum_{k_1'=0}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\binom{k_1-1}{k_1'}\cdots\binom{k_d-1}{k_d'}(-1)^{k_1'+\cdots+k_d'}\Bigg(\\
&\quad \delta\Big(D_{l_1,n_1}\ldots D_{l_{i-1},n_{i-1}}\Big)\Big(-\operatorname{ad}(b_0)\Big)^{n_i}\Big(\Big[D_{k_1-k_1',m_1}\ldots D_{k_d-k_d',m_d}, D_{l_i+k_1'+\cdots+k_d',0}\Big]\Big)\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \cdot D_{l_{i+1},n_{i+1}}\ldots D_{l_e,n_e}\\
&\quad + D_{l_1,n_1}\ldots D_{l_{i-1},n_{i-1}}\Big(-\operatorname{ad}(b_0)\Big)^{n_i}\Big(\Big[\delta\Big(D_{k_1-k_1',m_1}\ldots D_{k_d-k_d',m_d}\Big), D_{l_i+k_1'+\cdots+k_d',0}\Big]\Big)\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \cdot D_{l_{i+1},n_{i+1}}\ldots D_{l_e,n_e}\\
&\quad + D_{l_1,n_1}\ldots D_{l_{i-1},n_{i-1}}\Big(-\operatorname{ad}(b_0)\Big)^{n_i}\Big(\Big[D_{k_1-k_1',m_1}\ldots D_{k_d-k_d',m_d}, \delta(D_{l_i+k_1'+\cdots+k_d',0})\Big]\Big)\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \cdot D_{l_{i+1},n_{i+1}}\ldots D_{l_e,n_e}\\
&\quad + D_{l_1,n_1}\ldots D_{l_{i-1},n_{i-1}}\Big(-\operatorname{ad}(b_0)\Big)^{n_i}\Big(\Big[D_{k_1-k_1',m_1}\ldots D_{k_d-k_d',m_d}, D_{l_i+k_1'+\cdots+k_d',0}\Big]\Big)\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \cdot \delta\Big(D_{l_{i+1},n_{i+1}}\ldots D_{l_e,n_e}\Big)\Bigg)\\
&= d^q_{\delta(f)}(g) + d^q_f(\delta(g)).
\end{aligned}
$$

Moreover, we have

$$\delta\Big([f,g]\Big) = [\delta(f),g] + [f,\delta(g)].$$

Combining both formulas, we obtain

$$\delta\Big(\{f,g\}^D_q\Big) = \{\delta(f),g\}^D_q + \{f,\delta(g)\}^D_q.$$

□

The depth-graded double shuffle Lie algebra $\mathfrak{ls}$ (Definition B.36) defined for multiple zeta values embeds into the Lie algebra $\mathfrak{lq}$ via the associated depth-graded map of θ (obtained in Theorem 4.28).

Theorem 4.69. *We have an injective Lie algebra morphism*

$$
\begin{aligned}
\theta^D : (\mathfrak{ls}, \{-,-\}) &\hookrightarrow (\mathfrak{lq}, \{-,-\}^D_q),\\
\psi &\mapsto \theta^{\text{anti}}_{\mathcal{X}}(\psi) + \theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi)).
\end{aligned}
$$

The map $\Pi_{\mathcal{Y}}$ is given in Definition B.27.

It is expected that $\mathfrak{ls} \simeq \operatorname{gr}_D \mathfrak{dm}_0$, thus the image of the map θ^D should be contained in the associated depth-graded space $\mathfrak{lb}$ to $\mathfrak{bm}_0$.

Proof. First, observe that the maps $\theta_{\mathcal{X}}$ and $\theta_{\mathcal{Y}}$ also give injective Hopf algebra morphisms

$$
\begin{aligned}
\theta_{\mathcal{X}} : (\mathbb{Q}\langle\mathcal{X}\rangle, \text{conc}, \Delta_{ш}) &\to (\mathbb{Q}\langle\mathcal{B}\rangle, \text{conc}, \Delta_{ш}),\ x_0 \mapsto b_0,\ x_1 \mapsto b_1,\\
\theta_{\mathcal{Y}} : (\mathbb{Q}\langle\mathcal{Y}\rangle, \text{conc}, \Delta_{ш,\mathcal{Y}}) &\to (\mathbb{Q}\langle\mathcal{B}\rangle, \text{conc}, \Delta_{ш}),\ y_i \mapsto b_i \qquad i \geq 1.
\end{aligned}
$$

Let $\psi \in \mathfrak{ls}$. First, deduce from $(\psi \mid x_0) = 0$ that $(\theta^D(\psi) \mid b_0) = 0$. Since ψ is primitive for $\Delta_{ш}$, $\Pi_{\mathcal{Y}}(\psi)$ is primitive for $\Delta_{ш,\mathcal{Y}}$ and $\theta^{\text{anti}}_{\mathcal{X}},\ \theta_{\mathcal{Y}}$ are coalgebra morphisms, we obtain

$$
\begin{aligned}
\Delta_{ш}(\theta^D(\psi)) &= \Delta_{ш}\Big(\theta^{\text{anti}}_{\mathcal{X}}(\psi) + \theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi))\Big)\\
&= \mathbf{1}\otimes\theta^{\text{anti}}_{\mathcal{X}}(\psi) + \theta^{\text{anti}}_{\mathcal{X}}(\psi)\otimes\mathbf{1} + \mathbf{1}\otimes\theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi)) + \theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi))\otimes\mathbf{1}\\
&= \mathbf{1}\otimes\theta^D(\psi) + \theta^D(\psi)\otimes\mathbf{1}.
\end{aligned}
$$

Applying Lemma 4.20 and observing that $\Pi_0\Big(\theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi))\Big) = \theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi))$, we compute

$$\begin{aligned}\tau\Big(\Pi_0(\theta^D(\psi))\Big) &= \tau\Big(\Pi_0(\theta^{\mathrm{anti}}_{\mathcal{X}}(\psi))\Big) + \tau\Big(\theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi))\Big) = \theta_{\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi)) + \Pi_0(\theta^{\mathrm{anti}}_{\mathcal{X}}(\psi)) \\ &= \Pi_0(\theta^D(\psi)).\end{aligned}$$

Finally, we deduce from $(\psi \mid x_0^{k-1}x_1) = 0$ that $(\theta^D(\psi) \mid b_k) = 0$ for $k = 2, 4, 6$. Altogether, the map θ^D is well-defined and the injectivity follows immediately from the injectivity of $\theta^{\mathrm{anti}}_{\mathcal{X}}$ and $\theta_{\mathcal{Y}}$. ☐

Recall that we expect (Conjecture 1.23 (ii))

$$\begin{aligned}H_{\mathcal{U}(\mathfrak{lb})}(x,y) &= \sum_{w,d\geq 0} \dim \mathcal{U}(\mathfrak{lb})^{(w,d)} x^w y^d \\ &\overset{?}{=} \frac{1}{1 - a_1(x)y + a_2(x)y^2 - a_3(x)y^3 - a_4(x)y^4 + a_5(x)y^5}.\end{aligned}$$

Lemma 4.70. *There are numbers $g_{w,d} \in \mathbb{Z}$ satisfying*

$$\frac{1}{1 - a_1(x)y + a_2(x)y^2 - a_3(x)y^3 - a_4(x)y^4 + a_5(x)y^5} = \prod_{w,d\geq 1} (1 - x^w y^d)^{-g_{w,d}}.$$

Proof. Apply [Bou89, p. 140, Lemma 1]. ☐

If we assume that $\Big(1 - a_1(x)y + a_2(x)y^2 - a_3(x)y^3 - a_4(x)y^4 + a_5(x)y^5\Big)^{-1}$ is the Hilbert-Poincare series of $\mathcal{U}(\mathfrak{lb})$, then by Proposition A.35 and Corollary A.7 we must have $g_{w,d} \geq 0$ for all $w, d \geq 1$. In particular, Conjecture 1.23 (ii) is equivalent to

Conjecture 4.71. *For all $w, d \geq 1$, we have*

$$\dim_{\mathbb{Q}} \mathfrak{lb}^{(w,d)} = g_{w,d}.$$

The numbers $g_{w,d}$ are computed numerically in [BK20] as

$g_{w,d}$	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1													
2	0	0												
3	2	0	0											
4	0	1	0	0										
5	3	0	1	0	0									
6	0	2	0	1	0	0								
7	4	0	3	0	1	0	0							
8	0	7	0	3	0	1	0	0						
9	5	0	8	0	4	0	1	0	0					
10	0	12	0	11	0	4	0	1	0	0				
11	6	0	22	0	14	0	5	0	1	0	0			
12	0	20	0	31	0	17	0	5	0	1	0	0		
13	7	0	47	0	44	0	21	0	6	0	1	0	0	
14	0	31	0	81	0	58	0	25	0	6	0	1	0	0

Theorem 4.72. *For $w, d \leq 13$, we have*

$$\dim_{\mathbb{Q}} \mathfrak{lb}^{(w,d)} = g_{w,d}.$$

Proof. Take the depth-graded parts from the elements computed in Theorem 4.43. ☐

4.9 Supplement: A variant of the balanced quasi-shuffle Hopf algebra

For multiple zeta values there exists the shuffle Hopf algebra (Proposition B.14), which describes their product structure and is defined on some finite alphabet $\mathcal{X}$. For the balanced multiple q-zeta values there exists also such a finite alphabet. More precisely, let $\mathbb{Q}\langle p, y\rangle$ be the free non-commutative algebra generated by the letters p, y, denote the empty word by $\mathbf{1}$, and set $\mathbb{Q}\langle p, y\rangle^0 = \mathbb{Q}\mathbf{1} + p\mathbb{Q}\langle p, y\rangle y$. By Theorem 2.64 there is a surjective algebra morphism

$$\begin{aligned}(\mathbb{Q}\langle p, y\rangle^0, ⧢_q) &\to (\mathcal{Z}_q, \cdot), \\ p^{s_1}y \dots p^{s_l}y &\mapsto \zeta_q(s_1, \dots, s_l),\end{aligned} \tag{4.72.1}$$

where the product $⧢_q$ is recursively defined by $\mathbf{1} ⧢_q w = w ⧢_q \mathbf{1} = w$ and

$$\begin{aligned}(yu) ⧢_q v = u ⧢_q (yv) &= y(u ⧢_q v), \\ (pu) ⧢_q (pv) &= p(u ⧢_q pv) + p(pu ⧢_q v) + \begin{cases} p(u ⧢_q v), & \text{if } u = y\tilde{u} \text{ and } v = y\tilde{v}, \\ 0 & \text{else} \end{cases}\end{aligned}$$

for all $u, v, w \in \mathbb{Q}\langle p, y\rangle$. In this subsection, we will equip the algebra $(\mathbb{Q}\langle p, y\rangle, ⧢_q)$ with a graded bialgebra structure and obtain its completed dual. We will see that the Hopf algebra $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\text{dec}})$ (Theorem 4.2) embeds into this bialgebra. To give a better description of the bialgebra structure, we modify the algebra $(\mathbb{Q}\langle p, y\rangle, ⧢_q)$.

Definition 4.73. Denote by $\mathbb{Q}\langle p, c, y\rangle$ the free algebra over $\mathbb{Q}$ generated by the letters p, c, y and define

$$\mathcal{H}_q^+ = {}^{\mathbb{Q}\langle p, c, y\rangle}\big/_{\mathbb{Q}\langle p, c, y\rangle(py - c)\mathbb{Q}\langle p, c, y\rangle}.$$

In the following, we will identify $\mathcal{H}_q^+$ with the space generated by all words in the letters p, c, y, which do not contain the subword py. In particular, if we write $pw \in \mathcal{H}_q^+$, then we always assume $w \in \mathcal{H}_q^+ \backslash y\mathcal{H}_q^+$. Moreover, set

$$\mathcal{H}_q = (\mathcal{H}_q^+ \backslash y\mathcal{H}_q^+) \cup \{0\}. \tag{4.73.1}$$

For a word $w \in \mathcal{H}_q^+$, the weight $\text{wt}(w)$ is defined to be the number of letters of w, i.e., for $k_1, \dots, k_{d+1} \geq 1,\ m_0, \dots, m_d \geq 0$ we have

$$\text{wt}(y^{m_0}p^{k_1-1}cy^{m_1} \dots p^{k_d-1}cy^{m_d}p^{k_{d+1}-1}) = k_1 + \dots + k_{d+1} - 1 + m_0 + \dots m_d,$$

and the depth $\text{dep}(w)$ is defined to be the number of c's contained in w, i.e.,

$$\text{dep}(y^{m_0}p^{k_1-1}cy^{m_1} \dots p^{k_d-1}cy^{m_d}p^{k_{d+1}-1}) = d.$$

The notions of weight and depth endow $\mathcal{H}_q^+$ with two compatible ascending filtrations.

Definition 4.74. Define the product $⧢_q$ on $\mathcal{H}_q^+$ recursively by $\mathbf{1} ⧢_q w = w ⧢_q \mathbf{1} = w$ and

$$\begin{aligned}yu ⧢_q v = u ⧢_q yv &= y(u ⧢_q v), \\ a_1u ⧢_q a_2v &= a_1(u ⧢_q a_2v) + a_2(a_1u ⧢_q v) + \delta_{(a_1,a_2),(c,c)}cy(u ⧢_q v),\end{aligned}$$

for all $u, v, w \in \mathcal{H}_q^+$ and $a_1, a_2 \in \{p, c\}$.

Proposition 4.75. *There is an algebra isomorphism*

$$\psi : (\mathcal{H}_q^+, ⧢_q) \to (\mathbb{Q}\langle p, y\rangle, ⧢_q)$$

induced by the assignment $p \mapsto p,\ y \mapsto y$ *and* $c \mapsto py$. *In particular,* $(\mathcal{H}_q^+, ⧢_q)$ *is an associative and commutative algebra.*

Proof. There is a short exact sequence

$$0 \longrightarrow \mathbb{Q}\langle p,c,y\rangle(py-c)\mathbb{Q}\langle p,c,y\rangle \longrightarrow \mathbb{Q}\langle p,c,y\rangle \xrightarrow{\widetilde{\psi}} \mathbb{Q}\langle p,y\rangle \longrightarrow 0,$$

where $\widetilde{\psi}$ is the algebra morphism (with respect to concatenation) defined by $\widetilde{\psi}(p) = p$, $\widetilde{\psi}(y) = y$ and $\widetilde{\psi}(c) = py$. This induces a vector space isomorphism

$$\psi : \mathcal{H}_q^+ \xrightarrow{\sim} \mathbb{Q}\langle p,y\rangle.$$

We show that ψ is an algebra isomorphism. For $u,v \in \mathcal{H}_q^+$, one obtains by induction on the weight

$$\begin{aligned}
\psi(cu) \sqcup\!\sqcup_q \psi(cv) &= py\psi(u) \sqcup\!\sqcup_q py\psi(v) \\
&= py(\psi(u) \sqcup\!\sqcup_q py\psi(v)) + py(py\psi(u) \sqcup\!\sqcup_q \psi(v)) + py^2(\psi(u) \sqcup\!\sqcup_q \psi(v)) \\
&= py(\psi(u) \sqcup\!\sqcup_q \psi(cv)) + py(\psi(cu) \sqcup\!\sqcup_q \psi(v)) + py^2(\psi(u) \sqcup\!\sqcup_q \psi(v)) \\
&= py\psi(u \sqcup\!\sqcup_q cv) + py\psi(cu \sqcup\!\sqcup_q v) + py^2\psi(u \sqcup\!\sqcup_q v) \\
&= \psi(c(u \sqcup\!\sqcup_q cv) + c(cu \sqcup\!\sqcup_q v) + cy(u \sqcup\!\sqcup_q v)) \\
&= \psi(cu \sqcup\!\sqcup_q cv).
\end{aligned}$$

The other cases are verified in a similar way. □

Remark 4.76. There is also a definition of the non-homogeneous product $\sqcup\!\sqcup_{\mathrm{SZ}}$ on $\mathcal{H}_q^+$ corresponding to the product $\sqcup\!\sqcup_{\mathrm{SZ}}$ on $\mathbb{Q}\langle p,y\rangle$ defined for SZ multiple q-zeta values (Proposition 2.18), such that there is an algebra isomorphism $(\mathcal{H}_q^+, \sqcup\!\sqcup_{\mathrm{SZ}}) \to (\mathbb{Q}\langle p,y\rangle, \sqcup\!\sqcup_{\mathrm{SZ}})$. We will omit the explicit description, since we are interested in weight-graded structures.

Definition 4.77. Let $\Delta : \mathcal{H}_q^+ \to \mathcal{H}_q^+ \otimes \mathcal{H}_q^+$ be the coproduct (with respect to the concatenation product) defined by $\Delta(\mathbf{1}) = \mathbf{1} \otimes \mathbf{1}$ and

$$\begin{aligned}
\Delta(aw) &= (a \otimes \mathbf{1})\Delta(w) + \mathbf{1} \otimes aw, & a = p,c,\ w \in \mathcal{H}_q^+, \\
\Delta(yw) &= (y \otimes \mathbf{1})\Delta(w), & w \in \mathcal{H}_q^+.
\end{aligned}$$

Example 4.78. One computes

$$\begin{aligned}
\Delta(pcy) &= pcy \otimes \mathbf{1} + p \otimes cy + \mathbf{1} \otimes pcy, \\
\Delta(pcy^2) &= pcy^2 \otimes \mathbf{1} + p \otimes cy^2 + \mathbf{1} \otimes pcy^2.
\end{aligned}$$

Theorem 4.79. *The tuple $(\mathcal{H}_q^+, \sqcup\!\sqcup_q, \Delta)$ is a (weight-)graded commutative bialgebra without a counit.*

Proof. By Proposition 4.75 the pair $(\mathcal{H}_q^+, \sqcup\!\sqcup_q)$ is a commutative algebra, thus we have to show the coassociativity of Δ and the compatibility of $\sqcup\!\sqcup_q$ and Δ. First, we will show the coassociativity of Δ by induction on the weight. Using Sweedler's notation

$$\Delta(w) = \sum_{(w)} w^{(1)} \otimes w^{(2)}$$

one obtains for each $w \in \mathcal{H}_q^+$

$$\begin{aligned}
((\Delta \otimes \mathrm{id}) \circ \Delta)(yw) &= (\Delta \otimes \mathrm{id})((y \otimes \mathbf{1})\Delta(w)) = \sum_{(w)} \Delta(yw^{(1)}) \otimes w^{(2)} \\
&= (y \otimes \mathbf{1} \otimes \mathbf{1}) \sum_{(w)} \Delta(w^{(1)}) \otimes w^{(2)} = (y \otimes \mathbf{1} \otimes \mathbf{1}) \sum_{(w)} w^{(1)} \otimes \Delta(w^{(2)}) \\
&= (\mathrm{id} \otimes \Delta)\Big(\sum_{(w)} yw^{(1)} \otimes w^{(2)}\Big) = (\mathrm{id} \otimes \Delta)((y \otimes \mathbf{1})\Delta(w)) \\
&= ((\mathrm{id} \otimes \Delta) \circ \Delta)(yw)
\end{aligned}$$

and for $a \in \{p, c\}$

$$\begin{aligned}
\big((\Delta \otimes \mathrm{id}) \circ \Delta\big)(aw) &= (\Delta \otimes \mathrm{id})\big((a \otimes \mathbf{1})\Delta(w) + \mathbf{1} \otimes aw\big) \\
&= \sum_{(w)} \Delta(aw^{(1)}) \otimes w^{(2)} + \mathbf{1} \otimes \mathbf{1} \otimes aw \\
&= (a \otimes \mathbf{1} \otimes \mathbf{1}) \sum_{(w)} \Delta(w^{(1)}) \otimes w^{(2)} + \sum_{(w)} \mathbf{1} \otimes aw^{(1)} \otimes w^{(2)} + \mathbf{1} \otimes \mathbf{1} \otimes aw \\
&= (a \otimes \mathbf{1} \otimes \mathbf{1}) \sum_{(w)} w^{(1)} \otimes \Delta(w^{(2)}) + \mathbf{1} \otimes \big(\sum_{(w)} aw^{(1)} \otimes w^{(2)} + \mathbf{1} \otimes aw\big) \\
&= (\mathrm{id} \otimes \Delta)\big(\sum_{(w)} aw^{(1)} \otimes w^{(2)}\big) + \mathbf{1} \otimes \Delta(aw) \\
&= (\mathrm{id} \otimes \Delta)\big(\sum_{(w)} aw^{(1)} \otimes w^{(2)} + \mathbf{1} \otimes aw\big) \\
&= \big((\mathrm{id} \otimes \Delta) \circ \Delta\big)(aw).
\end{aligned}$$

In both cases, the fourth step follows from the induction hypotheses. Next, we prove the compatibility of the product $⧢_q$ and the coproduct Δ by induction on the weight. For $u, v \in \mathcal{H}_q^+$, compute

$$\begin{aligned}
\Delta(yu) ⧢_q \Delta(v) &= \big((y \otimes \mathbf{1})\Delta(u)\big) ⧢_q \Delta(v) = \sum_{(u),(v)} \big(yu^{(1)} ⧢_q v^{(1)}\big) \otimes \big(u^{(2)} ⧢_q v^{(2)}\big) \\
&= \sum_{(u),(v)} y\big(u^{(1)} ⧢_q v^{(1)}\big) \otimes \big(u^{(2)} ⧢_q v^{(2)}\big) = (y \otimes \mathbf{1})\big(\Delta(u) ⧢_q \Delta(v)\big) \\
&= (y \otimes \mathbf{1})\Delta(u ⧢_q v) = \Delta\big(y(u ⧢_q v)\big) = \Delta(yu ⧢_q v)
\end{aligned}$$

and similarly, obtain

$$\Delta(u) ⧢_q \Delta(yv) = \Delta(u ⧢_q yv).$$

For $a_1, a_2 \in \{p, c\}$ and $u, v \in \mathcal{H}_q^+$, one has

$$\begin{aligned}
\Delta(a_1u) ⧢_q \Delta(a_2v) &= \big((a_1 \otimes \mathbf{1})\Delta(u) + \mathbf{1} \otimes a_1u\big) ⧢_q \big((a_2 \otimes \mathbf{1})\Delta(v) + \mathbf{1} \otimes a_2v\big) \\
&= \sum_{(u),(v)} \big(a_1u^{(1)} ⧢_q a_2v^{(1)}\big) \otimes \big(u^{(2)} ⧢_q v^{(2)}\big) \\
&\quad + \sum_{(u)} a_1u^{(1)} \otimes \big(u^{(2)} ⧢_q a_2v\big) + \sum_{(v)} a_2v^{(1)} \otimes \big(a_1u ⧢_q v^{(2)}\big) \\
&\quad + \mathbf{1} \otimes \big(a_1u ⧢_q a_2v\big) \\
&= (a_1 \otimes \mathbf{1})\big(\Delta(u) ⧢_q (a_2 \otimes \mathbf{1})\Delta(v) + \Delta(u) ⧢_q (\mathbf{1} \otimes a_2v)\big) \\
&\quad + (a_2 \otimes \mathbf{1})\big((a_1 \otimes \mathbf{1})\Delta(u) ⧢_q \Delta(v) + (\mathbf{1} \otimes a_1u) ⧢_q \Delta(v)\big) \\
&\quad + \delta_{(a_1,a_2),(c,c)}(cy \otimes \mathbf{1})\big(\Delta(u) ⧢_q \Delta(v)\big) + \mathbf{1} \otimes \big(a_1u ⧢_q a_2v\big) \\
&= (a_1 \otimes \mathbf{1})\big(\Delta(u) ⧢_q \Delta(a_2v)\big) + (a_2 \otimes \mathbf{1})\big(\Delta(a_1u) ⧢_q \Delta(v)\big) \\
&\quad + \delta_{(a_1,a_2),(c,c)}(cy \otimes \mathbf{1})\big(\Delta(u) ⧢_q \Delta(v)\big) + \mathbf{1} \otimes \big(a_1u ⧢_q a_2v\big) \\
&= (a_1 \otimes \mathbf{1})\Delta(u ⧢_q a_2v) + \mathbf{1} \otimes \big(a_1(u ⧢_q a_2v)\big) \\
&\quad + (a_2 \otimes \mathbf{1})\Delta(a_1u ⧢_q v) + \mathbf{1} \otimes \big(a_2(a_1u ⧢_q v)\big) \\
&\quad + \delta_{(a_1,a_2),(c,c)}\Big((cy \otimes \mathbf{1})\Delta(u ⧢_q v) + \mathbf{1} \otimes \big(cy(u ⧢_q v)\big)\Big)
\end{aligned}$$

$$
\begin{aligned}
&= \Delta\big(a_1(u \sqcup\!\sqcup_q a_2v) + a_2(a_1u \sqcup\!\sqcup_q v) + \delta_{(a_1,a_2),(c,c)}cy(u \sqcup\!\sqcup_q v)\big)\\
&= \Delta(a_1u \sqcup\!\sqcup_q a_2v).
\end{aligned}
$$

A counit $\varepsilon : \mathcal{H}_q^+ \to \mathbb{Q}$ must satisfy $\big((\varepsilon \otimes \mathrm{id}) \circ \Delta\big)(y) = y$. Since

$$
\big((\varepsilon \otimes \mathrm{id}) \circ \Delta\big)(y) = (\varepsilon \otimes \mathrm{id})(y \otimes \mathbf{1}) = \varepsilon(y) \cdot \mathbf{1} \in \mathbb{Q}\mathbf{1},
$$

a counit cannot exist. □

Restricting to $\mathcal{H}_q$ (defined in (4.73.1)) yields a Hopf algebra isomorphic to the balanced quasi-shuffle Hopf algebra $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}})$ (Theorem 4.2).

Corollary 4.80. *The tuple $(\mathcal{H}_q, \sqcup\!\sqcup_q, \Delta)$ is a weight-graded commutative Hopf algebra. Moreover, the map*

$$
\begin{aligned}
\psi^{-1} \circ \tau \circ i : (\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}}) &\to (\mathcal{H}_q, \sqcup\!\sqcup_q, \Delta),\\
b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d} &\mapsto p^{m_d} cy^{k_d-1} \dots p^{m_1} cy^{k_1-1} p^{m_0},
\end{aligned}
$$

where $k_1, \dots, k_{d+1} \geq 1$ and $m_1, \dots, m_d \geq 0$, is an algebra isomorphism and a coalgebra anti isomorphism.

In particular, if the coproduct Δ gets replaced by $t \circ \Delta$, where t simply swaps the tensor product factors (see (A.14.1)), then $\psi^{-1} \circ \tau \circ i$ would be a Hopf algebra isomorphism.

Proof. Evidently, the maps $\sqcup\!\sqcup_q$ and Δ preserve the space $\mathcal{H}_q$ and a counit $\varepsilon : \mathcal{H}_q \to \mathbb{Q}$ is given by

$$
\varepsilon(w) = \begin{cases} 1, & \text{if } w = \mathbf{1} \\ 0 & \text{else} \end{cases}
$$

for each word $w \in \mathcal{H}_q$. So $(\mathcal{H}_q, \sqcup\!\sqcup_q, \Delta)$ is a connected bialgebra and hence a Hopf algebra (Theorem A.33).

As observed in (2.63.1), the map $\tau \circ i$ is an injective algebra morphism. Since ψ is an algebra isomorphism (Proposition 4.75), also $\psi^{-1} \circ \tau \circ i$ is an injective algebra morphism. Clearly, $\psi^{-1} \circ \tau \circ i$ is also surjective and hence an algebra isomorphism. Thus, we only have to check the compatibility of the coproducts Δ_{dec} and Δ under the morphism $\psi^{-1} \circ \tau \circ i$. For a word $w = b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}$, one computes

$$
\begin{aligned}
&\Big((\psi^{-1} \circ \tau \circ i) \otimes (\psi^{-1} \circ \tau \circ i)\Big) \circ \Delta_{\mathrm{dec}}(w)\\
&= \sum_{j=0}^{d} \sum_{i=0}^{m_j} (\psi^{-1} \circ \tau \circ i)(b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_j} b_0^{i}) \otimes (\psi^{-1} \circ \tau \circ i)(b_0^{m_j-i} b_{k_{j+1}} b_0^{m_{j+1}} \dots b_{k_d} b_0^{m_d})\\
&= \sum_{j=0}^{d} \sum_{i=0}^{m_j} p^i cy^{k_j-1} \dots p^{m_1} cy^{k_1-1} p^{m_0} \otimes p^{m_d} cy^{k_d-1} \dots p^{m_{j+1}} cy^{k_{j+1}-1} p^{m_j-i}\\
&= t \circ \Delta(p^{m_d} cy^{k_d-1} \dots p^{m_1} cy^{k_1-1} p^{m_0})\\
&= t \circ \Delta \circ (\psi^{-1} \circ \tau \circ i)(w)
\end{aligned}
$$

□

Next, we will determine a completed dual to the graded bialgebra $(\mathcal{H}_q^+, \sqcup\!\sqcup_q, \Delta)$. For any commutative $\mathbb{Q}$-algebra R with unit, denote $\mathcal{H}_q^+(R) = \mathcal{H}_q^+ \otimes_{\mathbb{Q}} R$. Let $\widehat{\mathcal{H}_q^+}(R)$ be the completion of $\mathcal{H}_q^+(R)$ with respect to the weight (Proposition A.45), i.e.,

$$
\widehat{\mathcal{H}_q^+}(R) = \prod_{w \geq 0} \mathcal{H}_q^+(R)^{(w)},
$$

where $\mathcal{H}_q^+(R)^{(w)}$ denotes the homogeneous subspace of $\mathcal{H}_q^+(R)$ of weight w. The space $\widehat{\mathcal{H}_q^+}(R)$ is filtered by weight and depth. Similarly, denote by $\widehat{\mathcal{H}_q}(R)$ the completion of the vector space $\mathcal{H}_q(R) = \mathcal{H}_q \otimes_{\mathbb{Q}} R$.

Definition 4.81. Define the product $\mathrm{conc}_y : \widehat{\mathcal{H}_q^+}(R) \otimes \widehat{\mathcal{H}_q^+}(R) \to \widehat{\mathcal{H}_q^+}(R)$ by

$$\mathrm{conc}_y(u \otimes v) = \begin{cases} uv, & v \neq y\tilde{v} \\ 0 & else \end{cases}$$

for all words $u, v \in \mathcal{H}_q^+$ and extend this definition R-linearly to the completion.

Definition 4.82. Define the coproduct $\Delta_{\sqcup\!\sqcup}^q : \widehat{\mathcal{H}_q^+}(R) \to \widehat{\mathcal{H}_q^+}(R) \otimes \widehat{\mathcal{H}_q^+}(R)$ by

$$\begin{aligned} \Delta_{\sqcup\!\sqcup}^q(a) &= \mathbf{1} \otimes a + a \otimes \mathbf{1}, \qquad a = p, c, \\ \Delta_{\sqcup\!\sqcup}^q(y^m) &= \mathbf{1} \otimes y^m + y^m \otimes \mathbf{1} + \sum_{i=1}^{m-1} y^i \otimes y^{m-i}, \\ \Delta_{\sqcup\!\sqcup}^q(cy^m) &= \mathbf{1} \otimes cy^m + cy^m \otimes \mathbf{1} + \sum_{i=1}^{m} cy^{i-1} \otimes cy^{m-i}, \end{aligned}$$

and extend this definition with respect to the product conc_y.

Theorem 4.83. *The tuple $(\widehat{\mathcal{H}_q^+}(R), \mathrm{conc}_y, \Delta_{\sqcup\!\sqcup}^q)$ is a complete cocommutative bialgebra without unit. The pairing*

$$\begin{aligned} \widehat{\mathcal{H}_q^+}(R) \otimes_{\mathbb{Q}} \mathcal{H}_q^+ &\to R, \\ \Phi \otimes w &\mapsto (\Phi \mid w), \end{aligned}$$

where $(\Phi \mid w)$ denotes the coefficient of $\Phi \in \widehat{\mathcal{H}_q^+}(R)$ in $w \in \mathcal{H}_q^+$, gives a duality between the weight-graded bialgebra $(\mathcal{H}_q^+, \sqcup\!\sqcup_q, \Delta)$ and the complete bialgebra $(\widehat{\mathcal{H}_q^+}(R), \mathrm{conc}_y, \Delta_{\sqcup\!\sqcup}^q)$.

Proof. We prove the duality of $(\mathcal{H}_q^+, \sqcup\!\sqcup_q, \Delta)$ and $(\widehat{\mathcal{H}_q^+}(R), \mathrm{conc}_y, \Delta_{\sqcup\!\sqcup}^q)$ with respect to the given pairing. Then $(\widehat{\mathcal{H}_q^+}(R), \mathrm{conc}_y, \Delta_{\sqcup\!\sqcup}^q)$ is a cocommutative bialgebra without a unit (cf Theorem A.31). For $f, g \in \widehat{\mathcal{H}_q^+}(R)$ and any word $w = a_1 \dots a_n \in \mathcal{H}_q^+$, one has

$$(\mathrm{conc}_y(f \otimes g), w) = \Big(f \otimes g \,\Big|\, \sum_{\substack{i=1 \\ a_i \neq y}}^{n+1} a_1 \dots a_{i-1} \otimes a_i \dots a_n\Big) = (f \otimes g \mid \Delta(w)).$$

So conc_y and Δ are dual maps. For $u, v \in \mathcal{H}_q^+$ and $a \in \{p, c\}$, one obtains

$$(\Delta_{\sqcup\!\sqcup}^q(a) \mid u \otimes v) = (\mathbf{1} \otimes a + a \otimes \mathbf{1} \mid u \otimes v) = (a \mid u \sqcup\!\sqcup_q v).$$

The last equality holds, since the word a appears in the product $u \sqcup\!\sqcup_q v$ if and only if $u = \mathbf{1},\ v = a$ or $u = a,\ v = \mathbf{1}$. Similarly, one has for $m \geq 1$

$$\begin{aligned} (\Delta_{\sqcup\!\sqcup}^q(y^m) \mid u \otimes v) &= \Big(\mathbf{1} \otimes y^m + y^m \otimes \mathbf{1} + \sum_{i=1}^{m-1} y^i \otimes y^{m-i} \,\Big|\, u \otimes v\Big) = (y^m \mid u \sqcup\!\sqcup_q v), \\ (\Delta_{\sqcup\!\sqcup}^q(cy^m) \mid u \otimes v) &= \Big(\mathbf{1} \otimes cy^m + cy^m \otimes \mathbf{1} + \sum_{i=1}^{m} cy^{i-1} \otimes cy^{m-i} \,\Big|\, u \otimes v\Big) = (cy^m \mid u \sqcup\!\sqcup_q v). \end{aligned}$$

Since $\Delta_{\sqcup\!\sqcup}^{q}$ is compatible with conc_y by definition and we proved that

$$(\Delta_{\sqcup\!\sqcup}^{q}(f) \mid u \otimes v) = (f \mid u \sqcup\!\sqcup_q v)$$

holds on the algebra generators of $(\widehat{\mathcal{H}_q^+}(R), \mathrm{conc}_y)$, the maps $\Delta_{\sqcup\!\sqcup}^{q}$ and $\sqcup\!\sqcup_q$ are dual. □

The complete dual balanced quasi-shuffle Hopf algebra $(R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q)$ (Theorem 4.5) embeds into the dual bialgebra $(\widehat{\mathcal{H}_q^+}(R), \mathrm{conc}_y, \Delta_{\sqcup\!\sqcup}^{q})$.

Corollary 4.84. *The tuple $(\widehat{\mathcal{H}_q}(R), \mathrm{conc}, \Delta_{\sqcup\!\sqcup}^{q})$ is a complete, cocommutative Hopf algebra. Moreover, the map*

$$\begin{aligned}\psi^{-1} \circ \tau \circ i : (R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q) &\to (\widehat{\mathcal{H}_q}(R), \mathrm{conc}, \Delta_{\sqcup\!\sqcup}^{q}),\\ b_0^{m_0} b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d} &\mapsto p^{m_d} c y^{k_d-1} \dots p^{m_1} c y^{k_1-1} p^{m_0},\end{aligned}$$

where $k_1, \dots, k_{d+1} \geq 1$ and $m_1, \dots, m_d \geq 0$, is an algebra anti isomorphism and a coalgebra isomorphism.

In particular, if $\widehat{\mathcal{H}_q}(R)$ is equipped instead of conc with the product $\mathrm{conc} \circ t$ (see (A.14.1) for the definition of t), then $\psi^{-1} \circ \tau \circ i$ would be a Hopf algebra isomorphism.

Proof. The product conc_y restricted to $\widehat{\mathcal{H}_q}(R)$ is simply the concatenation product. In particular, there is a unit given by $\mathbf{1}$. So $(\widehat{\mathcal{H}_q}(R), \mathrm{conc}, \Delta_{\sqcup\!\sqcup}^{q})$ is a connected bialgebra and thus a Hopf algebra (Theorem A.33).
Since $(\mathbb{Q}\langle\mathcal{B}\rangle, *_q, \Delta_{\mathrm{dec}})$, $(R\langle\langle\mathcal{B}\rangle\rangle, \mathrm{conc}, \Delta_q)$ and $(\mathcal{H}_q, \sqcup\!\sqcup_q, \Delta)$, $(\widehat{\mathcal{H}_q}(R), \mathrm{conc}, \Delta_{\sqcup\!\sqcup}^{q})$ are graded dual Hopf algebras, Corollary 4.80 implies that the map $\psi^{-1} \circ \tau \circ i$ is an algebra anti isomorphism and a coalgebra isomorphism. □

5 Lie algebras for $\mathcal{Z}_q$: Commutative approach

For multiple zeta values there exists also an approach to Lie algebras using Ecalle's theory of moulds ([Ec11],[Sc15]), which is presented in Appendix B.3. In this section, we will relate the algebra $\mathcal{Z}_q$ of multiple q-zeta values to (conjectural) Lie algebras consisting of bimoulds. A basic introduction to the theory of bimoulds is given in Appendix C. We will end this section by comparing the commutative approach presented in this section to the non-commutative one given in Section 4.

5.1 The space $\mathrm{BARI}^{\mathbb{Q},\mathrm{pol}}_{\underline{\mathrm{il}},\mathrm{swap}}$ and the uri bracket

A spanning set for the algebra $\mathcal{Z}_q$ of multiple q-zeta values is given by the combinatorial bi-multiple Eisenstein series

$$G\binom{k_1,\dots,k_d}{m_1,\dots,m_d},\quad k_1,\dots,k_d\geq 1,\ m_1,\dots,m_d\geq 0.$$

For $k+m\geq 2$ even, the combinatorial bi-Eisenstein series $G\binom{k}{m}$ is essentially the m-th derivative of the classical Eisenstein series of weight k expressed in its Fourier expansion (cf Example 2.48 1)). In particular, the algebra $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$ of quasi-modular forms with rational coefficients is contained in $\mathcal{Z}_q$.
Consider the bimould $\mathfrak{G}=(\mathfrak{G}_d)_{d\geq 0}\in\mathrm{GBARI}^{\mathrm{pow},\mathcal{Z}_q}$ of the generating series of the combinatorial bi-multiple Eisenstein series, so $\mathfrak{G}_0=1$ and

$$\mathfrak{G}_d\begin{pmatrix}X_1,\dots,X_d\\ Y_1,\dots,Y_d\end{pmatrix}=\sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}} G\begin{pmatrix}k_1,\dots,k_d\\ m_1,\dots,m_d\end{pmatrix}X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\dots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}.$$

By Theorem 2.46, the bimould $\mathfrak{G}$ is symmetril and swap invariant. Conjecturally, all algebraic relations in $\mathcal{Z}_q$ can be deduced from these two properties of the bimould $\mathfrak{G}$ (Conjecture 2.51).

The main idea to obtain a Lie algebra is to consider the bimould $\mathfrak{G}$ of the generating series of the combinatorial bi-multiple Eisenstein series modulo products and quasi-modular forms.

Definition 5.1. Let $\mathcal{Z}_q^{(w)}$ be the homogeneous space spanned by all combinatorial bi-multiple Eisenstein series of weight w. Moreover, set

$$\overline{\mathcal{Z}}_q=\mathcal{Z}_q\big/\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))\mathcal{Z}_q$$

and for each $w\geq 0$ denote by $\overline{\mathcal{Z}}_q^{(w)}$ the image of the homogeneous subspace $\mathcal{Z}_q^{(w)}$ in $\overline{\mathcal{Z}}_q$. Then let $\mathcal{I}_q=\bigoplus_{w\geq 1}\overline{\mathcal{Z}}_q^{(w)}$ and define the $\mathbb{Q}$-algebra

$$\mathcal{T}_q=\mathcal{I}_q\big/\mathcal{I}_q^2.$$

By construction, the algebra $\mathcal{T}_q$ is graded by weight and all products become trivial. Moreover, the dimension of the homogeneous subspace $\mathcal{T}_q^{(w)}$ of weight w is equal to the number of algebra generators of $\mathcal{Z}_q\big/\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))\mathcal{Z}_q$ in weight w.

Let $\overline{G}\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$ be the image of the combinatorial bi-multiple Eisenstein series $G\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$ in $\mathcal{T}_q$ and consider their generating series for each $d \geq 1$,

$$\overline{\mathfrak{G}}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d \geq 1 \\ m_1,\dots,m_d \geq 0}} \overline{G}\begin{pmatrix} k_1,\dots,k_d \\ m_1,\dots,m_d \end{pmatrix} X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\dots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}.$$

Set $\overline{\mathfrak{G}}_0 = 0$, then $\overline{\mathfrak{G}} = (\overline{\mathfrak{G}}_d)_{d\geq 0}$ is a bimould contained in $\mathrm{BARI}^{\mathrm{pow},\mathcal{T}_q}$.

Theorem 5.2. *The bimould $\overline{\mathfrak{G}}$ is contained in the space*

$$\mathrm{BARI}^{\mathrm{pow},\mathcal{T}_q}_{\underline{\mathrm{il}},\mathrm{swap}} = \left\{ A \in \mathrm{BARI}^{\mathrm{pow},\mathcal{T}_q} \;\middle|\; \begin{array}{l} \cdot\ A \textit{ is alternil}, \\ \cdot\ A \textit{ is swap invariant}, \\ \cdot\ A_1\binom{X_1}{Y_1} \textit{ is even} \end{array} \right\}.$$

Proof. Alternility is symmetrility modulo products, thus we deduce from the symmetrility of $\mathfrak{G}$ (Theorem 2.46) that $\overline{\mathfrak{G}}$ is alternil. The swap invariance of $\mathfrak{G}$ gives only linear relations among the combinatorial bi-multiple Eisenstein series, thus the image $\overline{\mathfrak{G}}$ is still swap invariant. The combinatorial bi-Eisenstein series $G\binom{k}{m}$ for $k+m \geq 2$ even are exactly the coefficients of the odd monomials in $\mathfrak{G}_1$. On the other hand, these combinatorial bi-Eisenstein series are essentially the classical Eisenstein series and their derivatives and hence are contained in $\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$ (Example 2.48, 1)). Thus their images in $\mathcal{T}_q$ vanish and $\overline{\mathfrak{G}}_1$ is even. □

Corollary 5.3. *Decompose the bimould $\overline{\mathfrak{G}}$ as*

$$\overline{\mathfrak{G}} = \sum_{\alpha} \alpha \cdot \xi^{\alpha},$$

where α runs through a vector space basis of $\mathcal{T}_q$. Then any bimould ξ^{α} is contained in

$$\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}} = \left\{ A \in \mathrm{BARI}^{\mathrm{pow},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}} \;\middle|\; \begin{array}{l} \cdot\ A_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} \in \mathbb{Q}[X_1,Y_1,\dots,X_d,Y_d] \textit{ for all } d \geq 1, \\ \cdot\ A_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} \neq 0 \textit{ only for finitely many } d \geq 1 \end{array} \right\}.$$

Proof. Since $\overline{\mathfrak{G}}$ is contained in $\mathrm{BARI}^{\mathrm{pow},\mathcal{T}_q}_{\underline{\mathrm{il}},\mathrm{swap}}$ (Theorem 5.2) and we decompose over a $\mathbb{Q}$-vector space basis of $\mathcal{T}_q$, evidently, the bimoulds ξ^{α} are contained in $\mathrm{BARI}^{\mathrm{pow},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$. Since $\mathcal{T}_q$ is graded by weight and all homogeneous components $\mathcal{T}_q^{(w)}$ are finite-dimensional, the entries of ξ^{α} must be polynomials. Moreover, the depth is bounded by the weight, thus only finitely many components of ξ^{α} can be non-zero. □

Example 5.4. There are the following bimoulds in $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$, which should correspond to the elements $\overline{G}\binom{3}{0},\ \overline{G}\binom{2}{1},\ \overline{G}\binom{5}{0},\ \overline{G}\binom{4}{1},\ \overline{G}\binom{3}{2},\ \overline{G}\binom{2,1,1}{1,0,0} \in \mathcal{T}_q$

$$\xi\begin{pmatrix} 3 \\ 0 \end{pmatrix} = (X_1^2 + Y_1^2,\ X_1 - 2X_2 - Y_1 + Y_2,\ \frac{1}{3},\ 0,\ \dots),$$

$$\xi\begin{pmatrix} 2 \\ 1 \end{pmatrix} = (X_1Y_1,\ -X_1 + X_2 - Y_2,\ 0,\ \dots),$$

$$\xi\binom{5}{0} = (X_1^4+Y_1^4,\ 2X_1^3-3X_2^3+\frac{9}{2}X_1X_2^2-\frac{11}{2}X_1^2X_2-2Y_1^3-\frac{1}{2}Y_1^2Y_2+\frac{1}{2}Y_1Y_2^2+2Y_2^3,$$
$$2X_1^2-\frac{1}{2}X_2^2-\frac{1}{2}X_3^2-\frac{11}{2}X_1X_2+\frac{9}{2}X_1X_3+2X_2X_3+2Y_1^2-4Y_2^2+2Y_3^2$$
$$-\frac{3}{2}Y_1Y_2+3Y_1Y_3-\frac{3}{2}Y_2Y_3,\ X_1-4X_2+6X_3-4X_4-Y_1+3Y_2-3Y_3+Y_4,$$
$$\frac{1}{5},\ 0,\ \dots),$$

$$\xi\binom{4}{1} = (X_1^3Y_1+X_1Y_1^3,\ -X_1^3+X_2^3-\frac{3}{2}X_1X_2^2+\frac{3}{2}X_1^2X_2-Y_2^3-\frac{3}{2}Y_1^2Y_2-\frac{3}{2}Y_1Y_2^2$$
$$-2X_1X_2Y_1+X_1X_2Y_2+X_2Y_1Y_2-X_1Y_1Y_2+X_1^2Y_1-X_1^2Y_2+2X_2Y_2^2-X_1Y_2^2$$
$$+X_2Y_1^2-2X_1Y_1^2-2X_2^2Y_2,\ -X_1^2+\frac{3}{2}X_2^2+\frac{1}{2}X_1X_2+\frac{3}{2}X_1X_3-2X_2X_3-\frac{1}{2}X_3^2$$
$$+Y_2^2-Y_3^2+\frac{3}{2}Y_1Y_2-\frac{3}{2}Y_2Y_3+6X_2Y_3-6X_1Y_3-5X_3Y_1+3X_3Y_2+X_2Y_2$$
$$+4X_2Y_1,\ X_1-4X_2+4X_3-X_4+Y_2-3Y_3+Y_4,\ 0,\ \dots),$$
$$\xi\binom{3}{2} = (X_1^2Y_1^2,\ X_1X_2Y_1-X_1X_2Y_2-\frac{3}{2}X_1^2Y_1+\frac{3}{2}X_2^2Y_2-X_1Y_1Y_2-X_2Y_1Y_2+\frac{1}{2}X_1Y_1^2$$
$$-X_2Y_1^2-\frac{3}{2}X_2Y_2^2,\ \frac{1}{2}X_1^2-X_2^2+\frac{1}{2}X_3^2+X_1X_2-2X_1X_3+X_2X_3+\frac{1}{2}Y_2^2+\frac{1}{2}Y_3^2$$
$$+2Y_2Y_3+\frac{1}{2}X_1Y_1-4X_2Y_3+\frac{9}{2}X_1Y_3+\frac{7}{2}X_3Y_1-2X_3Y_2-\frac{1}{2}X_2Y_2+\frac{1}{2}X_1Y_2$$
$$-\frac{5}{2}X_2Y_1,\ -X_1+\frac{7}{2}X_2-4X_3+\frac{3}{2}X_4-\frac{3}{2}Y_2+\frac{5}{2}Y_3-Y_4,\ 0,\ \dots),$$
$$\xi\binom{2,1,1}{1,0,0} = (0,\ 0,\ X_1Y_1+3X_1Y_3-3X_2Y_1-2X_2Y_2-3X_2Y_3+3X_3Y_1+X_3Y_3,$$
$$-X_1+3X_2-3X_3+X_4-Y_2+2Y_3-Y_4,\ 0,\ \dots).$$

The space $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ is graded by weight, and the homogeneous components $\big(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\big)^{(w)}$ are obtained from (C.24.1).

Corollary 5.5. *For each $w\geq 1$, one has*

$$\dim_{\mathbb{Q}}\mathcal{T}_q^{(w)}\leq \dim_{\mathbb{Q}}\big(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\big)^{(w)}.$$

Proof. If α is a basis element of $\mathcal{T}_q^{(w)}$, then by Corollary 5.3 the bimould ξ^α is contained in $\big(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\big)^{(w)}$. In particular, the dimension of the space spanned by the ξ^α, where α is homogeneous of weight w, is bounded by the dimension of $\big(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\big)^{(w)}$. As the assignment $\alpha\mapsto\xi^\alpha$ is injective, also the dimension of $\mathcal{T}_q^{(w)}$ is bounded by $\dim_{\mathbb{Q}}\big(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\big)^{(w)}$. □

Conjecturally the space $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ has a weight-graded Lie algebra structure and the dimensions of the homogeneous subspaces are compatible with the dimension conjecture 1.21. More precisely, this means

Conjecture 5.6. *([Kü19]) (i) There is a decomposition of graded algebras*

$$\mathcal{Z}_q\simeq\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))\otimes\mathcal{U}\big(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\big)^\vee.$$

(ii) For all $w\geq 1$, the following holds

$$\dim_{\mathbb{Q}}\mathcal{T}_q^{(w)}=\dim_{\mathbb{Q}}\big(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\big)^{(w)}=g_w,$$

where the numbers g_w are defined in Lemma 4.41.

It is hard to attack this conjecture with the computer even for low weights, since the occurring polynomials are very large.

The rest of this subsection is devoted to explain the conjectural Lie algebra structure on the subspace $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$, which was suggested by L. Schneps. This will be done more generally for some fixed commutative $\mathbb{Q}$-algebra R with unit. In particular, we will always omit the index indicating the underlying $\mathbb{Q}$-algebra in the following.

Definition 5.7. For any bimould $B \in \mathrm{GBARI}^{\mathrm{fL}}$, define the automorphism ganit_B of $\mathrm{BARI}^{\mathrm{fL}}$ by

$$\mathrm{ganit}_B(A)(\mathbf{w}) = \sum_{\substack{\mathbf{w}=\mathbf{a}_1\mathbf{b}_1\ldots\mathbf{a}_s\mathbf{b}_s \\ \mathbf{a}_1,\mathbf{b}_1,\ldots,\mathbf{b}_{s-1},\mathbf{a}_s\neq\emptyset}} = A(\mathbf{a}_1\rfloor\ldots\mathbf{a}_s\rfloor)B(\lceil\mathbf{b}_1)\ldots B(\lceil\mathbf{b}_s),$$

where the flexions are explained in Appendix C.2. Moreover, let $\mathrm{pic},\mathrm{poc} \in \mathrm{GBARI}^{\mathrm{fL}}$ be the bimoulds for $d \geq 1$ given by

$$\mathrm{pic}\begin{pmatrix} X_1,\ldots,X_d \\ Y_1,\ldots,Y_d \end{pmatrix} = \frac{1}{X_1\ldots X_d}, \qquad \mathrm{poc}\begin{pmatrix} X_1,\ldots,X_d \\ Y_1,\ldots,Y_d \end{pmatrix} = -\frac{1}{X_1(X_1-X_2)\ldots(X_{d-1}-X_d)}.$$

Example 5.8. For any bimould $A \in \mathrm{BARI}^{\mathrm{fL}}$, one obtains

$$\mathrm{ganit}_{\mathrm{pic}}(A)\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2 \end{pmatrix} = A\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2 \end{pmatrix} + \frac{1}{X_2-X_1}A\begin{pmatrix} X_1 \\ Y_1+Y_2 \end{pmatrix},$$

$$\begin{aligned}\mathrm{ganit}_{\mathrm{pic}}(A)\begin{pmatrix} X_1,X_2,X_3 \\ Y_1,Y_2,Y_3 \end{pmatrix} &= A\begin{pmatrix} X_1,X_2,X_3 \\ Y_1,Y_2,Y_3 \end{pmatrix} + \frac{1}{X_3-X_2}A\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2+Y_3 \end{pmatrix} \\ &+ \frac{1}{X_2-X_1}A\begin{pmatrix} X_1,X_3 \\ Y_1+Y_2,Y_3 \end{pmatrix} + \frac{1}{(X_2-X_1)(X_3-X_1)}A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix},\end{aligned}$$

$$\begin{aligned}\mathrm{ganit}_{\mathrm{pic}}(A)\begin{pmatrix} X_1,X_2,X_3,X_4 \\ Y_1,Y_2,Y_3,Y_4 \end{pmatrix} &= A\begin{pmatrix} X_1,X_2,X_3,X_4 \\ Y_1,Y_2,Y_3,Y_4 \end{pmatrix} + \frac{1}{X_4-X_3}A\begin{pmatrix} X_1,X_2,X_3 \\ Y_1,Y_2,Y_3+Y_4 \end{pmatrix} \\ &+ \frac{1}{X_3-X_2}A\begin{pmatrix} X_1,X_2,X_4 \\ Y_1,Y_2+Y_3,Y_4 \end{pmatrix} + \frac{1}{X_2-X_1}A\begin{pmatrix} X_1,X_3,X_4 \\ Y_1+Y_2,Y_3,Y_4 \end{pmatrix} \\ &+ \frac{1}{(X_3-X_2)(X_4-X_2)}A\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2+Y_3+Y_4 \end{pmatrix} + \frac{1}{(X_2-X_1)(X_3-X_1)}A\begin{pmatrix} X_1,X_4 \\ Y_1+Y_2+Y_3,Y_4 \end{pmatrix} \\ &+ \frac{1}{(X_2-X_1)(X_4-X_3)}A\begin{pmatrix} X_1,X_3 \\ Y_1+Y_2,Y_3+Y_4 \end{pmatrix} \\ &+ \frac{1}{(X_2-X_1)(X_3-X_1)(X_4-X_1)}A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3+Y_4 \end{pmatrix},\end{aligned}$$

$$\mathrm{ganit}_{\mathrm{poc}}(A)\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2 \end{pmatrix} = A\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2 \end{pmatrix} - \frac{1}{X_2-X_1}A\begin{pmatrix} X_1 \\ Y_1+Y_2 \end{pmatrix},$$

$$\begin{aligned}\mathrm{ganit}_{\mathrm{poc}}(A)\begin{pmatrix} X_1,X_2,X_3 \\ Y_1,Y_2,Y_3 \end{pmatrix} &= A\begin{pmatrix} X_1,X_2,X_3 \\ Y_1,Y_2,Y_3 \end{pmatrix} - \frac{1}{X_3-X_2}A\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2+Y_3 \end{pmatrix} \\ &- \frac{1}{X_2-X_1}A\begin{pmatrix} X_1,X_3 \\ Y_1+Y_2,Y_3 \end{pmatrix} - \frac{1}{(X_2-X_1)(X_2-X_3)}A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix},\end{aligned}$$

$$\begin{aligned}
\operatorname{ganit}_{\mathrm{poc}}(A)\begin{pmatrix} X_1, X_2, X_3, X_4 \\ Y_1, Y_2, Y_3, Y_4 \end{pmatrix} &= A\begin{pmatrix} X_1, X_2, X_3, X_4 \\ Y_1, Y_2, Y_3, Y_4 \end{pmatrix} - \frac{1}{X_4 - X_3} A\begin{pmatrix} X_1, X_2, X_3 \\ Y_1, Y_2, Y_3 + Y_4 \end{pmatrix} \\
&- \frac{1}{X_3 - X_2} A\begin{pmatrix} X_1, X_2, X_4 \\ Y_1, Y_2 + Y_3, Y_4 \end{pmatrix} - \frac{1}{X_2 - X_1} A\begin{pmatrix} X_1, X_3, X_4 \\ Y_1 + Y_2, Y_3, Y_4 \end{pmatrix} \\
&- \frac{1}{(X_3 - X_2)(X_3 - X_4)} A\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 + Y_3 + Y_4 \end{pmatrix} - \frac{1}{(X_2 - X_1)(X_2 - X_3)} A\begin{pmatrix} X_1, X_4 \\ Y_1 + Y_2 + Y_3, Y_4 \end{pmatrix} \\
&+ \frac{1}{(X_2 - X_1)(X_4 - X_3)} A\begin{pmatrix} X_1, X_3 \\ Y_1 + Y_2, Y_3 + Y_4 \end{pmatrix} \\
&- \frac{1}{(X_2 - X_1)(X_2 - X_3)(X_3 - X_4)} A\begin{pmatrix} X_1 \\ Y_1 + Y_2 + Y_3 + Y_4 \end{pmatrix}.
\end{aligned}$$

Proposition 5.9. *([Bau14, Lemma 4.37, Proposition 4.38]) The map* $\operatorname{ganit}_{\mathrm{pic}}$ *restricts to a vector space isomorphism*

$$\operatorname{ganit}_{\mathrm{pic}} : \mathrm{BARI}_{\mathrm{al}}^{\mathrm{fL}} \to \mathrm{BARI}_{\mathrm{il}}^{\mathrm{fL}}.$$

The inverse map is given by $\operatorname{ganit}_{\mathrm{poc}}$. □

In Remark C.18 it is explained how to extend the definition of alternality and alternility to the space $\mathrm{BARI}^{\mathrm{fL}}$.

L. Schneps suggested the following definition for a Lie bracket.

Definition 5.10. For bimoulds $A, B \in \mathrm{BARI}^{\mathrm{fL}}$, define the uri bracket as

$$\operatorname{uri}(A, B) = \operatorname{ganit}_{\mathrm{pic}}\Big(\operatorname{ari}\Big(\operatorname{ganit}_{\mathrm{poc}}(A), \operatorname{ganit}_{\mathrm{poc}}(B)\Big)\Big).$$

Since $\Big(\mathrm{BARI}_{\mathrm{al}}^{\mathrm{fL}}, \operatorname{ari}\Big)$ is a Lie algebra (Theorem C.24), one obtains from Proposition 5.9 the following.

Theorem 5.11. *The space* $\mathrm{BARI}_{\mathrm{il}}^{\mathrm{fL}}$ *equipped with the uri bracket is a Lie algebra.*

We are interested in a polynomial expression of the uri bracket, since this would prove that the uri bracket preserves the space $\mathrm{BARI}^{\mathrm{pow}}$. More precisely, we define the following analog of the derivation arit (Definition C.20).

Definition 5.12. For two bimoulds $A, B \in \mathrm{BARI}^{\mathrm{pow}}$ and $d, e, r \geq 1$ define $\operatorname{urit}_B(A)^{(d,e,r)}$ to be the bimould, whose only nontrivial component is in depth $d + e + r$ and is given by

$$\begin{aligned}
&\operatorname{urit}_B(A)^{(d,e,r)}\begin{pmatrix} X_1, \dots, X_{d+e+r} \\ Y_1, \dots, Y_{d+e+r} \end{pmatrix} \\
&\quad = \sum_{i=1}^{e} A_e\begin{pmatrix} X_1, \dots, X_{i-1}, X_i, X_{i+1+d+r}, \dots, X_{d+e+r} \\ Y_1, \dots, Y_{i-1}, Y_i + \dots + Y_{i+d+r}, Y_{i+1+d+r}, \dots, Y_{d+e+r} \end{pmatrix} \\
&\qquad \cdot \Bigg[\sum_{\substack{0 \leq s \leq r-1 \\ \text{or} \\ s = d+r}} \prod_{\substack{0 \leq k \leq r-1,\ k \neq s \\ \text{or} \\ k = d+r,\ k \neq s}} \frac{1}{(X_{i+k} - X_{i+s})} B_d\begin{pmatrix} X_{i+r} - X_{i+s}, \dots, X_{i+d+r-1} - X_{i+s} \\ Y_{i+r}, \dots, Y_{i+d+r-1} \end{pmatrix} \\
&\qquad\qquad - \sum_{s=0}^{r} \prod_{\substack{k=0 \\ k \neq s}}^{r} \frac{1}{(X_{i+k} - X_{i+s})} B_d\begin{pmatrix} X_{i+1+r} - X_{i+s}, \dots, X_{i+d+r} - X_{i+s} \\ Y_{i+1+r}, \dots, Y_{i+d+r} \end{pmatrix} \Bigg].
\end{aligned}$$

Then we define the bimould $\mathrm{urit}_B(A)$ by

$$\mathrm{urit}_B(A)\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} = \mathrm{arit}_B(A)\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} + \sum_{\substack{d+e+r=n \\ d,e,r\geq 1}} \mathrm{urit}_B(A)^{(d,e,r)}\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix}.$$

Example 5.13. Let $A, B \in \mathrm{BARI}^{\mathrm{pow}}$, then one obtains

$$\mathrm{urit}_B(A)\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} = \mathrm{arit}_B(A)\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix},$$

$$\begin{aligned}
\mathrm{urit}_B(A)\begin{pmatrix} X_1, X_2, X_3 \\ Y_1, Y_2, Y_3 \end{pmatrix} &= \mathrm{arit}_B(A)\begin{pmatrix} X_1, X_2, X_3 \\ Y_1, Y_2, Y_3 \end{pmatrix} \\
&\quad + A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix} \frac{1}{X_3 - X_1}\left(B\begin{pmatrix} X_2 - X_1 \\ Y_2 \end{pmatrix} - B\begin{pmatrix} X_2 - X_3 \\ Y_2 \end{pmatrix}\right) \\
&\quad - A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix} \frac{1}{X_2 - X_1}\left(B\begin{pmatrix} X_3 - X_1 \\ Y_3 \end{pmatrix} - B\begin{pmatrix} X_3 - X_2 \\ Y_3 \end{pmatrix}\right),
\end{aligned}$$

$$\begin{aligned}
&\mathrm{urit}_B(A)\begin{pmatrix} X_1, X_2, X_3, X_4 \\ Y_1, Y_2, Y_3, Y_4 \end{pmatrix} = \mathrm{arit}_B(A)\begin{pmatrix} X_1, X_2, X_3, X_4 \\ Y_1, Y_2, Y_3, Y_4 \end{pmatrix} \\
&+ A\begin{pmatrix} X_1, X_4 \\ Y_1+Y_2+Y_3, Y_4 \end{pmatrix}\left[\frac{1}{X_3 - X_1}\left(B\begin{pmatrix} X_2 - X_1 \\ Y_2 \end{pmatrix} - B\begin{pmatrix} X_2 - X_3 \\ Y_2 \end{pmatrix}\right)\right. \\
&\qquad\qquad \left. - \frac{1}{X_2 - X_1}\left(B\begin{pmatrix} X_3 - X_1 \\ Y_3 \end{pmatrix} - B\begin{pmatrix} X_3 - X_2 \\ Y_3 \end{pmatrix}\right)\right] \\
&+ A\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2+Y_3+Y_4 \end{pmatrix}\left[\frac{1}{X_4 - X_2}\left(B\begin{pmatrix} X_3 - X_2 \\ Y_3 \end{pmatrix} - B\begin{pmatrix} X_3 - X_4 \\ Y_3 \end{pmatrix}\right)\right. \\
&\qquad\qquad \left. - \frac{1}{X_3 - X_2}\left(B\begin{pmatrix} X_4 - X_2 \\ Y_4 \end{pmatrix} - B\begin{pmatrix} X_4 - X_3 \\ Y_4 \end{pmatrix}\right)\right] \\
&+ A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3+Y_4 \end{pmatrix}\left[\frac{1}{X_4 - X_1}\left(B\begin{pmatrix} X_2 - X_1, X_3 - X_1 \\ Y_2, Y_3 \end{pmatrix} - B\begin{pmatrix} X_2 - X_4, X_3 - X_4 \\ Y_2, Y_3 \end{pmatrix}\right)\right. \\
&\qquad\qquad \left. - \frac{1}{X_2 - X_1}\left(B\begin{pmatrix} X_3 - X_1, X_4 - X_1 \\ Y_3, Y_4 \end{pmatrix} - B\begin{pmatrix} X_3 - X_2, X_4 - X_2 \\ Y_3, Y_4 \end{pmatrix}\right)\right] \\
&+ A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3+Y_4 \end{pmatrix}\left[\frac{1}{(X_2 - X_1)(X_4 - X_1)} B\begin{pmatrix} X_3 - X_1 \\ Y_3 \end{pmatrix}\right. \\
&\qquad\qquad \left. + \frac{1}{(X_1 - X_2)(X_4 - X_2)} B\begin{pmatrix} X_3 - X_2 \\ Y_3 \end{pmatrix} + \frac{1}{(X_1 - X_4)(X_2 - X_4)} B\begin{pmatrix} X_3 - X_4 \\ Y_3 \end{pmatrix}\right] \\
&- A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3+Y_4 \end{pmatrix}\left[\frac{1}{(X_2 - X_1)(X_3 - X_1)} B\begin{pmatrix} X_4 - X_1 \\ Y_4 \end{pmatrix}\right. \\
&\qquad\qquad \left. + \frac{1}{(X_1 - X_2)(X_3 - X_2)} B\begin{pmatrix} X_4 - X_2 \\ Y_4 \end{pmatrix} + \frac{1}{(X_1 - X_3)(X_2 - X_3)} B\begin{pmatrix} X_4 - X_3 \\ Y_4 \end{pmatrix}\right].
\end{aligned}$$

Proposition 5.14. *For all* $A, B \in \mathrm{BARI}^{\mathrm{pow}}$*, one has* $\mathrm{urit}_B(A) \in \mathrm{BARI}^{\mathrm{pow}}$.

Proof. By [St99, Excercise 7.4.], for some commutative variables $a_1, \dots, a_r$ the following holds

$$\sum_{\substack{j_1+\cdots+j_r=m+1\\ j_1,\dots,j_r\geq 1}} a_1^{j_1-1}\dots a_r^{j_r-1} = \sum_{s=1}^{r}\prod_{\substack{k=1\\ k\neq s}}^{r}\frac{1}{(a_s-a_k)}a_s^m. \tag{5.14.1}$$

Let $B \in \mathrm{BARI}^{\mathrm{pow}}$ be a bimould. Without loss of generality, assume that

$$B_d\begin{pmatrix} X_1,\dots,X_d\\ Y_1,\dots,Y_d\end{pmatrix} = X_1^{k_1-1}\dots X_d^{k_d-1}Y_1^{m_1}\dots Y_d^{m_d}$$

for some $k_1,\dots,k_d \geq 1,\ m_1,\dots,m_d\geq 0$. Then we obtain for each $i\geq 1$

$$\begin{aligned}
&\sum_{s=0}^{r}\prod_{\substack{k=0\\ k\neq s}}^{r}\frac{1}{(X_{i+k}-X_{i+s})}B_d\begin{pmatrix} X_{i+1+r}-X_{i+s},\dots,X_{i+d+r}-X_{i+s}\\ Y_{i+1+r},\dots,Y_{i+d+r}\end{pmatrix}\\
&= Y_{i+1+r}^{m_1}\dots Y_{i+d+r}^{m_d}\sum_{\substack{l_1=0\\ (l_1,\dots,l_d)\neq(0,\dots,0)}}^{k_1-1}\cdots\sum_{l_d=0}^{k_d-1}\binom{k_1-1}{l_1}\cdots\binom{k_d-1}{l_d}(-1)^{l_1+\cdots+l_d}\\
&\qquad\qquad \cdot X_{i+1+r}^{k_1-l_1-1}\dots X_{i+d+r}^{k_d-l_d-1}\sum_{s=0}^{r}\prod_{\substack{k=0\\ k\neq s}}^{r}\frac{1}{(X_{i+k}-X_{i+s})}X_{i+s}^{l_1+\cdots+l_d}\\
&\overset{(5.14.1)}{=} Y_{i+1+r}^{m_1}\dots Y_{i+d+r}^{m_d}\sum_{\substack{l_1=0\\ (l_1,\dots,l_d)\neq(0,\dots,0)}}^{k_1-1}\cdots\sum_{l_d=0}^{k_d-1}\binom{k_1-1}{l_1}\cdots\binom{k_d-1}{l_d}(-1)^{l_1+\cdots+l_d+r}\\
&\qquad\qquad \cdot\sum_{\substack{j_1+\cdots+j_{r+1}=l_1+\cdots+l_d+1\\ j_1,\dots,j_{r+1}\geq 1}} X_{i+1+r}^{k_1-l_1-1}\dots X_{i+d+r}^{k_d-l_d-1}X_i^{j_1-1}\dots X_{i+r}^{j_{r+1}-1}.
\end{aligned}$$

A completely analogous calculation shows that also the poles in the first sum in the definition of urit_B (Definition 5.12) cancel out. □

Definition 5.15. For bimoulds $A, B \in \mathrm{BARI}^{\mathrm{pow}}$, define the bimould $\mathrm{preuri}(A,B) \in \mathrm{BARI}^{\mathrm{pow}}$ by

$$\mathrm{preuri}(A,B) = \mathrm{urit}_A(B) + \mathrm{mu}(B,A).$$

We expect that preuri is exactly a pre-Lie multiplication for the uri bracket, which means

Conjecture 5.16. *For all bimoulds $A, B\in \mathrm{BARI}^{\mathrm{pow}}$ the following holds*

$$\mathrm{uri}(A,B) = \mathrm{preuri}(A,B) - \mathrm{preuri}(B,A).$$

In particular, Proposition 5.14 would imply that the uri bracket preserves the space $\mathrm{BARI}^{\mathrm{pow}}$.

Proposition 5.17. *(i) For depth $d\leq 6$ Conjecture 5.16 holds, in particular for depth $d \leq 6$ the space $\mathrm{BARI}^{\mathrm{pow}}$ is preserved by* uri*.*

(ii) For depth $d\leq 3$, the Lie bracket uri *preserves the swap invariant bimoulds in $\mathrm{BARI}_{\mathrm{il}}^{\mathrm{pow}}$.*

Proof. (i) This was calculated explicitly with the computer algebra system Maple.
(ii) is obtained in [SK]. □

Example 5.18. From Example 5.13, one can easily obtain explicit formulas for uri in low depths. E.g., we obtain for $A, B \in \mathrm{BARI}^{\mathrm{pow}}$ that

$$\begin{aligned}
\mathrm{uri}(A,B)\begin{pmatrix} X_1, X_2, X_3 \\ Y_1, Y_2, Y_3 \end{pmatrix} &= \mathrm{ari}(A,B)\begin{pmatrix} X_1, X_2, X_3 \\ Y_1, Y_2, Y_3 \end{pmatrix} \\
&+ B\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix} \frac{1}{X_3 - X_1}\left(A\begin{pmatrix} X_2 - X_1 \\ Y_2 \end{pmatrix} - A\begin{pmatrix} X_2 - X_3 \\ Y_2 \end{pmatrix}\right) \\
&- B\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix} \frac{1}{X_2 - X_1}\left(A\begin{pmatrix} X_3 - X_1 \\ Y_3 \end{pmatrix} - A\begin{pmatrix} X_3 - X_2 \\ Y_3 \end{pmatrix}\right) \\
&- A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix} \frac{1}{X_3 - X_1}\left(B\begin{pmatrix} X_2 - X_1 \\ Y_2 \end{pmatrix} - B\begin{pmatrix} X_2 - X_3 \\ Y_2 \end{pmatrix}\right) \\
&+ A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix} \frac{1}{X_2 - X_1}\left(B\begin{pmatrix} X_3 - X_1 \\ Y_3 \end{pmatrix} - B\begin{pmatrix} X_3 - X_2 \\ Y_3 \end{pmatrix}\right).
\end{aligned}$$

It is conjectured in [SK] that uri is well-behaved for alternility and swap invariance in all depths, in particular, this leads to the following.

Conjecture 5.19. *([SK]) The space* $\mathrm{BARI}^{\mathrm{pow}}_{\underline{\mathrm{il}},\mathrm{swap}}$ *is a Lie algebra with the uri bracket.*

In particular, if Conjecture 5.19 holds, then the subspace $\mathrm{BARI}^{\mathrm{pol}}_{\underline{\mathrm{il}},\mathrm{swap}}$ equipped with the uri bracket would be a weight-graded Lie algebra. As stated in Proposition 5.17 the conjecture is proven up to depth 3 in [SK].

The space $\mathrm{BARI}^{\mathrm{pol}}_{\underline{\mathrm{il}},\mathrm{swap}}$ can be seen as a bi-version of the Lie algebra $\mathrm{ARI}^{\mathrm{pol}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ (introduced in Theorem B.45).

Theorem 5.20. *([SK]) There is a map* $\theta_{\mathrm{BIMU}} : \mathrm{ARI}^{\mathrm{pol}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}} \to \mathrm{BARI}^{\mathrm{pol}}_{\underline{\mathrm{il}},\mathrm{swap}}$ *given for each* $d \geq 1$ *by*

$$\theta_{\mathrm{BIMU}}(A)\begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix} = \mathrm{swap}(A)(X_1, \dots, X_d) + A(Y_1, \dots, Y_d) + C_A$$

where C_A *denotes the unique constant bimould, such that* $\mathrm{swap}(A) + C_A$ *is alternil.*
The image $\theta_{\mathrm{BIMU}}\left(\mathrm{ARI}^{\mathrm{pol}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}\right)$ *is a Lie algebra for the uri bracket. In particular, if Conjecture 5.19 holds, the map* θ_{BIMU} *is an embedding of graded Lie algebras.* □

5.2 The Lie algebra $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$

We study the depth-graded behavior of the bimould $\overline{\mathfrak{G}}$ of generating series of the combinatorial bi-multiple Eisenstein series modulo products and quasi-modular forms.

Definition 5.21. Denote by $\mathcal{M}_q$ the associated depth-graded algebra to $\mathcal{T}_q$ (Definition 5.1), so

$$\mathcal{M}_q = \bigoplus_{w,d\geq 1} \mathcal{M}_q^{(w,d)}, \qquad \mathcal{M}_q^{(w,d)} = {\mathrm{Fil}_D^{(d)}(\mathcal{T}_q^{(w)})}\Big/{\mathrm{Fil}_D^{(d-1)}(\mathcal{T}_q^{(w)})}.$$

In particular, $\mathcal{M}_q$ is a bi-graded algebra with respect to weight and depth. Moreover, the dimension of $\mathcal{M}_q^{(w,d)}$ equals the number of algebra generators of $\mathrm{gr}_D\, {\mathcal{Z}}\big/{\widetilde{\mathcal{M}}^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))\mathcal{Z}}$ in weight w and depth d.
Denote by $\mathrm{gr}_D\, \overline{G}\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$ the image of the combinatorial bi-multiple Eisenstein series $G\binom{k_1,\dots,k_d}{m_1,\dots,m_d}$ in $\mathcal{M}_q$ and consider their generating series in any fixed depth $d\geq 1$,

$$\mathrm{gr}_D\, \overline{\mathfrak{G}}_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d\end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}} \mathrm{gr}_D\, \overline{G}\begin{pmatrix} k_1,\dots,k_d \\ m_1,\dots,m_d\end{pmatrix} X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\dots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}.$$

Let $\mathrm{gr}_D\, \overline{\mathfrak{G}}_0 = 0$, then $\mathrm{gr}_D\, \overline{\mathfrak{G}} = (\mathrm{gr}_D\, \overline{\mathfrak{G}}_d)_{d\geq 0}$ is a bimould in $\mathrm{BARI}^{\mathrm{pow},\mathcal{M}_q}$.

Theorem 5.22. *The bimould $\mathrm{gr}_D\, \overline{\mathfrak{G}}$ is contained in*

$$\mathrm{BARI}^{\mathrm{pow},\mathcal{M}_q}_{\underline{\mathrm{al}},\mathrm{swap}} = \left\{ A\in \mathrm{BARI}^{\mathrm{pow},\mathcal{M}_q} \;\middle|\; \begin{array}{l} \cdot\ A \text{ is alternal,}\\ \cdot\ A \text{ is swap invariant,}\\ \cdot\ A_1\binom{X_1}{Y_1} \text{ is even}\end{array}\right\}.$$

Proof. By Theorem 5.2 the bimould $\overline{\mathfrak{G}}$ in contained in $\mathrm{BARI}^{\mathrm{pow},\mathcal{T}_q}_{\underline{\mathrm{il}},\mathrm{swap}}$. The definition of alternility considered modulo lower depth is just alternality and the swap operator is homogeneous in depth, thus the bimould $\mathrm{gr}_D\, \overline{\mathfrak{G}}$ is alternal and swap invariant. Moreover, $\overline{\mathfrak{G}}_1$ is an even function, thus the same holds for $\mathrm{gr}_D\, \overline{\mathfrak{G}}$. □

Corollary 5.23. *Decompose $\mathrm{gr}_D\, \overline{\mathfrak{G}}$ over a vector space basis of $\mathcal{M}_q$,*

$$\mathrm{gr}_D\, \overline{\mathfrak{G}} = \sum_\beta \beta\cdot \mathrm{gr}_D\, \xi^\beta.$$

Then any bimould $\mathrm{gr}_D\, \xi^\beta$ is contained in

$$\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}} = \left\{ A\in \mathrm{BARI}^{\mathrm{pow},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}} \;\middle|\; \begin{array}{l} \cdot\ A_d\begin{pmatrix} X_1,\dots,X_d\\ Y_1,\dots,Y_d\end{pmatrix} \in \mathbb{Q}[X_1,Y_1,\dots,X_d,Y_d] \text{ for all } d\geq 1,\\ \cdot\ A_d\begin{pmatrix} X_1,\dots,X_d\\ Y_1,\dots,Y_d\end{pmatrix} \neq 0 \text{ only for finitely many } d\geq 1\end{array}\right\}.$$

Proof. As in Corollary 5.3, this follows immediately from the weight-grading of $\mathcal{M}_q$. □

Example 5.24. For each $k\geq 1,\ m\geq 0$ and $k+m$ odd, the elements

$$\mathrm{gr}_D\, \xi\begin{pmatrix} k\\ m\end{pmatrix} = (X_1^m Y_1^m (X_1^{k-m-1} + Y_1^{k-m-1}),\ 0,\ \dots)$$

are contained in $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$. They should correspond to the elements $\mathrm{gr}_D\, \overline{G}\binom{k}{m} \in \mathcal{M}_q$.

The space $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$ is bi-graded by weight and depth, and the homogeneous components $\left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}\right)^{(w,d)}$ are given in (C.24.2).

Corollary 5.25. *For all $w, d \geq 1$, the following holds*

$$\dim_{\mathbb{Q}} \mathcal{M}_q^{(w,d)} \leq \dim_{\mathbb{Q}} \left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}\right)^{(w,d)}.$$

Proof. Apply the same arguments as in Corollary 5.5. □

Equality in Corollary 5.25 is not expected, this will be explained in the following.

Theorem 5.26. *([SS20, Theorem 3.1, Proposition 3.4 + 3.5]) For each commutative $\mathbb{Q}$-algebra R with unit, the space $\mathrm{BARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}},\mathrm{swap}}$ equipped with the ari bracket (Definition C.22) is a bi-graded Lie algebra.* □

Proposition 5.27. *Let R be a commutative $\mathbb{Q}$-algebra with unit and assume that the pair $(\mathrm{BARI}^{\mathrm{pol},R}_{\underline{\mathrm{il}},\mathrm{swap}}, \mathrm{uri})$ is a Lie algebra (Conjecture 5.19). Then the map*

$$\mathrm{gr}_D : (\mathrm{BARI}^{\mathrm{pol},R}_{\underline{\mathrm{il}},\mathrm{swap}}, \mathrm{uri}) \to (\mathrm{BARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}},\mathrm{swap}}, \mathrm{ari}),$$
$$(0, \ldots, 0, A_r, A_{r+1}, \ldots) \mapsto (0, \ldots, 0, A_r, 0, \ldots)$$

is a Lie algebra morphism.

Proof. Since the swap operator is homogeneous in depth and the map gr_D maps alternil bimoulds to alternal bimoulds (Proposition C.19), the map gr_D is well-defined. By definition, the associated depth-graded map to $\mathrm{ganit}_{\mathrm{pic}}$ and $\mathrm{ganit}_{\mathrm{poc}}$ is simply the identity. Thus, the associated depth-graded to the uri bracket (see Definition 5.10) is just the ari bracket. □

The map in Proposition 5.27 is not surjective, for example, one has

$$\dim_{\mathbb{Q}} \mathrm{gr}_D^{(2)} \left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\right)^{(8)} = 7 < 8 = \dim_{\mathbb{Q}} \left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}\right)^{(8,2)}. \tag{5.27.1}$$

In accordance with Conjecture 5.6, the following is expected.

Conjecture 5.28. *([Kü19])*
(i) The space $\mathrm{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ is a proper bi-graded Lie subalgebra of $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$.
(ii) For all $w, d \geq 1$, the following holds

$$\dim_{\mathbb{Q}} \mathrm{gr}_D^{(d)} \left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\right)^{(w)} = \dim_{\mathbb{Q}} \mathcal{M}_q^{(w,d)} = g_{w,d},$$

where the numbers $g_{w,d}$ are defined in Lemma 4.70.

Evidence for the dimension part of this conjecture was computed by U. Kühn up to weight 26 and depth 4. The example in (5.27.1) together with Conjecture 5.28 explains why equality in Corollary 5.25 is not expected.

The Lie algebra $\mathrm{BARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}},\mathrm{swap}}$ can be seen as a generalization of the Lie algebra $\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ of moulds (introduced in Theorem B.53).

Proposition 5.29. *([SK]) Let R be commutative $\mathbb{Q}$-algebra with unit. Then the map $\theta^D_{\mathrm{BIMU}} : (\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}, \mathrm{ari}) \to (\mathrm{BARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}},\mathrm{swap}}, \mathrm{ari})$ given by*

$$\theta^D_{\mathrm{BIMU}}(A)\begin{pmatrix} X_1, \ldots, X_d \\ Y_1, \ldots, Y_d \end{pmatrix} = \mathrm{swap}(A)(X_1, \ldots, X_d) + A(Y_1, \ldots, Y_d)$$

is an embedding of bi-graded Lie algebras.

Proof. By definition of the space $\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$, the bimould $\theta^D_{\mathrm{BIMU}}(A)$ is alternal. Moreover, one computes directly

$$\begin{aligned}
&\mathrm{swap}(\theta^D_{\mathrm{BIMU}}(A))\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}\\
&\quad=\mathrm{swap}(A)(Y_1+\dots+Y_d,\dots,Y_1+Y_2,Y_1)+A(X_d,X_{d-1}-X_d,\dots,X_1-X_2)\\
&\quad=A(Y_1,\dots,Y_d)+\mathrm{swap}(A)(X_1,\dots,X_d)\\
&\quad=\theta^D_{\mathrm{BIMU}}(A)\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}.
\end{aligned}$$

Thus $\theta^D_{\mathrm{BIMU}}(A)$ is contained in $\mathrm{BARI}^{\mathrm{pol},R}_{\mathrm{al,swap}}$ for all $A\in\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$. Finally, obtain for $A,B\in\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$

$$\begin{aligned}
&\mathrm{ari}(\theta^D_{\mathrm{BIMU}}(A),\theta^D_{\mathrm{BIMU}}(B))\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}\\
&\qquad=\mathrm{ari}(\mathrm{swap}(A),\mathrm{swap}(B))(X_1,\dots,X_d)+\mathrm{ari}(A,B)(Y_1,\dots,Y_d)\\
&\qquad=\mathrm{swap}\left(\mathrm{ari}(A,B)\right)(X_1,\dots,X_d)+\mathrm{ari}(A,B)(Y_1,\dots,Y_d)\\
&\qquad=\theta^D_{\mathrm{BIMU}}\left(\mathrm{ari}(A,B)\right)\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}
\end{aligned}$$

The first equality follows from $\mathrm{ari}(A,\mathrm{swap}(B))=0$, which is proven in [SK], and the second equality is a consequence of [Sc15, Lemma 2.4.1, 2.5.5.]. ☐

At the end of this subsection, we will explain the conjectured structure of the Lie algebra $(\mathrm{gr}_D\,\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}},\mathrm{ari})$ and relate this to the depth-graded dimension conjecture 1.21. In the following, we will work over the field $\mathbb{Q}$ for simplicity, but everything holds also for an arbitrary commutative $\mathbb{Q}$-algebra R with unit.

An immediate consequence of [Ec11, eq (2.79)] is the following parity result.

Proposition 5.30. *If $w,d\geq 1$ and $w\not\equiv d \mod 2$, then one has*

$$\left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}\right)^{(w,d)}=\{0\}.$$

☐

Proposition 5.31. *([Kü19]) The Lie algebra $(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}},\mathrm{ari})$ is equipped with the derivation $\delta:\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}\to\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$ given by*

$$\delta(A)\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}=(X_1Y_1+\dots+X_dY_d)A\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}.$$

☐

Definition 5.32. Denote by $\mathfrak{F}$ the Lie algebra over $\mathbb{Q}$ generated by the elements

$$\mathrm{gr}_D\,\xi\binom{k}{0}=\left(X_1^{k-1}+Y_1^{k-1},\ 0,\ \dots\right),\qquad k\geq 1\text{ odd},$$

and their derivatives

$$\delta^m\,\mathrm{gr}_D\,\xi\binom{k}{0}=\left((X_1Y_1)^m(X_1^{k-1}+Y_1^{k-1}),\ 0,\ \dots\right),\qquad k\geq 1\text{ odd},\ m\geq 0.$$

For each $A \in \operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ the component A_1 must be even and swap invariant. Thus, $\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ and $\mathfrak{F}$ must coincide in depth 1

$$\operatorname{gr}_D^{(1)} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}} = \mathfrak{F}^{(1)}.$$

In particular, if $\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ is a Lie algebra, then $\mathfrak{F}$ is a Lie subalgebra of $\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$. By Proposition 5.29 there is a Lie algebra embedding

$$\theta^D_{\mathrm{BIMU}} : \mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}} \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}\,.$$

For $k \geq 3$ odd, the elements $\operatorname{gr}_D \xi\binom{k}{0}$ lie in the image of θ^D_{BIMU}, since their preimages are exactly given by the generators $\operatorname{gr}_D \xi(k) = (X_1^{k-1},\ 0,\ \ldots)$ of $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ in depth 1 (cf Definition B.59). In particular, $\mathfrak{F}$ contains the images of the ekma moulds obtained for multiple zeta values,

$$\theta^D_{\mathrm{BIMU}}(\mathfrak{E}) \subset \mathfrak{F}.$$

Lemma 5.33. *The number f_w of generators of $\mathfrak{F}^{(1)}$ is given by*

$$\sum_{w \geq 1} f_w x^w = D(x) O_1(x) = a_1(x),$$

where $D(x) = \frac{1}{1-x^2}$, $O_1(x) = \frac{x}{1-x^2}$.

Proof. The generators $\operatorname{gr}_D \xi\binom{k}{0}$, $k \geq 1$ odd, are counted by the term $O_1(x)$ and their derivatives are counted by the term $D(x)$. ☐

Theorem 5.34. *([Kü19]) The number r_w of independent relations in $\mathfrak{F}^{(2)}$ of weight w is given by*

$$\sum_{w \geq 2} r_w x^w = D(x) \sum_{k \geq 4} \dim(\mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z})))^2 x^k = a_2(x),$$

where $D(x) = \frac{1}{1-x^2}$ and $\mathcal{M}_k(\mathrm{SL}_2(\mathbb{Z}))$ is the vector space of modular forms of weight k.

Sketch of proof.[7] Due to the shape of the ari bracket in depth 2 (Example C.23) and the generators of $\mathfrak{F}$, the number r_w is exactly given by the dimension of the space $\mathfrak{R}_w$ spanned by all homogeneous polynomials $P \in \mathbb{Q}[X_1, X_2, Y_1, Y_2]$ of degree $w-2$ satisfying the following relations

$$\begin{aligned}
&P\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} + P\begin{pmatrix} X_2, X_1 - X_2 \\ Y_1 + Y_2, Y_1 \end{pmatrix} + P\begin{pmatrix} X_2 - X_1, X_1 \\ Y_2, Y_1 + Y_2 \end{pmatrix} = 0,\\
&P\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} + P\begin{pmatrix} X_2, X_1 \\ Y_2, Y_1 \end{pmatrix} = 0,\\
&P\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} = P\begin{pmatrix} \pm X_1, X_2 \\ \pm Y_1, Y_2 \end{pmatrix} = P\begin{pmatrix} X_1, \pm X_2 \\ Y_1, \pm X_2 \end{pmatrix},\\
&P\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} = P\begin{pmatrix} Y_1, X_2 \\ X_1, Y_2 \end{pmatrix} = P\begin{pmatrix} X_1, Y_1 \\ Y_2, X_2 \end{pmatrix}.
\end{aligned}$$

The space $\mathfrak{R}_w$ can be decomposed as

$$\mathfrak{R}_w = \ker \Delta \oplus \delta(\mathfrak{R}_{w-2}),$$

[7]More details can be found in [Con22]

where $\Delta = \partial_{X_1}\partial_{Y_1} + \partial_{X_2}\partial_{Y_2}$ denotes the symplectic Laplacian. Following an idea of Zagier, the space $\ker\Delta$ can be identified with the space of all symmetric tensor products of even or odd period polynomials. This identification allows counting the dimensions of $\ker\Delta$ and one obtains the claimed formula. □

The relations in $\mathfrak{F}^{(2)}$ can be divided into two families. On the one hand, one obtains for all $k \geq 1$ odd

$$\operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}1\\0\end{pmatrix}, \operatorname{gr}_D \xi\begin{pmatrix}k\\0\end{pmatrix}\right) = 0 \tag{5.34.1}$$

and hence also

$$\delta^m \operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}1\\0\end{pmatrix}, \operatorname{gr}_D \xi\begin{pmatrix}k\\0\end{pmatrix}\right) = 0 \quad \text{for all } m \geq 0. \tag{5.34.2}$$

These relations are called the Eisenstein relations. On the other hand, there are the well-known period polynomial relations in $(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}})^{(2)}$ (Proposition B.60). Applying the embedding θ^D_{BIMU} (Proposition 5.29) leads to period polynomial relations between the generators $\operatorname{gr}_D \xi\binom{k}{0}$ for $k \geq 3$ odd. For example, one has in weight 12

$$\operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}3\\0\end{pmatrix}, \operatorname{gr}_D \xi\begin{pmatrix}9\\0\end{pmatrix}\right) - 3\operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}5\\0\end{pmatrix}, \operatorname{gr}_D \xi\begin{pmatrix}7\\0\end{pmatrix}\right) = 0. \tag{5.34.3}$$

There are also derivatives of these period polynomial relations.

The Eisenstein relations and the period polynomial relations induced by θ^D_{BIMU} intersect in depth 3. More precisely, consider any period polynomial relations induced by θ^D_{BIMU},

$$\sum \lambda_{k_1,k_2} \operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}k_1\\0\end{pmatrix}, \operatorname{gr}_D \xi\begin{pmatrix}k_2\\0\end{pmatrix}\right) = 0.$$

Then applying Jacobi's identity yields

$$\begin{aligned}\operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}1\\0\end{pmatrix}, \sum \lambda_{k_1,k_2} \operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}k_1\\0\end{pmatrix}, \operatorname{gr}_D \xi\begin{pmatrix}k_2\\0\end{pmatrix}\right)\right) = \\ \sum \lambda_{k_1,k_2} \operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}k_1\\0\end{pmatrix}, \operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}k_2\\0\end{pmatrix}, \operatorname{gr}_D \xi\begin{pmatrix}1\\0\end{pmatrix}\right)\right) \\ + \sum \lambda_{k_1,k_2} \operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}k_2\\0\end{pmatrix}, \operatorname{ari}\left(\operatorname{gr}_D \xi\begin{pmatrix}1\\0\end{pmatrix}, \operatorname{gr}_D \xi\begin{pmatrix}k_1\\0\end{pmatrix}\right)\right),\end{aligned}$$

and the right-hand side consists of Lie products of the Eisenstein relations. Evidently, there also exist derivatives of these intersections of relations. Denote by i_w the number of this kind of intersections in $\mathfrak{F}^{(3)}$ and weight w.

Lemma 5.35. *The following holds*

$$\sum_{i \geq 3} i_w x^w = D(x)xS(x) = a_3(x),$$

where $D(x) = \frac{1}{1-x^2}$, $S(x) = \frac{x^{12}}{(1-x^4)(1-x^6)}$.

Proof. The series $S(x)$ is exactly the Hilbert-Poincare series of the cusp forms $\mathcal{S}(\mathrm{Sl}_2(\mathbb{Z}))$ and thus counts the number of period polynomial relations induced by θ^D_{BIMU} (see Proposition B.60). Since the intersections of relations occur when considering the Lie product of these period polynomial relations and $\mathrm{gr}_D\, \xi\binom{1}{0}$, the series $S(x)$ needs to be multiplied by x. Finally, there exist derivations of the intersections of relations illustrated above, this is encoded in the term $D(x)$. $\square$

It is expected that there exist no new relations or intersections of relations in $\mathfrak{F}^{(w)}$ for $w > 3$. So the computations in Lemma 5.33, Theorem 5.34, and Lemma 5.35 lead to the following Hilbert-Poincare series of $\mathcal{U}(\mathfrak{F})$.

Conjecture 5.36. *([Kü19]) The Hilbert-Poincare series of the universal enveloping algebra of $\mathfrak{F}$ is given by*

$$H_{\mathcal{U}(\mathfrak{F})}(x,y) = \sum_{w,d\geq 0} \dim_{\mathbb{Q}} \mathcal{U}(\mathfrak{F})^{(w,d)} x^w y^d = \frac{1}{1 - a_1(x)y + a_2(x)y^2 - a_3(x)y^3}.$$

This conjecture is verified by U. Kühn up to weight 27 and depth 6.

In depth 4, the homogeneous subspace $\mathfrak{F}^{(4)}$ is properly included in $\mathrm{gr}_D^{(4)} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$. We will explain now a construction how to find these additional generators of $\mathrm{gr}_D^{(4)} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$, we call this Ecalle's construction (cf [Ec11, Section 7.3, 7.7]).

If $(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}, \mathrm{uri})$ is a Lie algebra (Conjecture 5.19), then $(\mathrm{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}, \mathrm{ari})$ is the associated depth-graded Lie algebra (cf Proposition 5.27). Thus, any relation in the Lie algebra $\mathfrak{F} \subset \mathrm{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ can be lifted to $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$. For example lifting the period polynomial relation induced by θ^D_{BIMU} given in (5.34.3) to $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$, one obtains

$$\mathrm{uri}\left(\xi\begin{pmatrix}3\\0\end{pmatrix}, \xi\begin{pmatrix}9\\0\end{pmatrix}\right) - 3\,\mathrm{uri}\left(\xi\begin{pmatrix}5\\0\end{pmatrix}, \xi\begin{pmatrix}7\\0\end{pmatrix}\right) = \xi_\Delta,$$

where $\xi_\Delta \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ is an element of depth ≥ 4. In general, lifting any relation in $\mathfrak{F}^{(2)}$ to a relation in $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$, the depth 2 part must vanish by construction and the depth 3 part vanishes by Proposition 5.30. Thus any relation in $\mathfrak{F}^{(2)}$ gives rise to an element in $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ of depth ≥ 4. Then apply the morphism in Proposition 5.27 to obtain a (possibly trivial) element in $\mathrm{gr}_D^{(4)} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$.

Definition 5.37. Let $\mathfrak{D}$ be the Lie algebra generated by the elements in $\mathrm{gr}_D^{(4)} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ induced by the relations in $\mathfrak{F}^{(2)}$ in the above explained way.

By construction, the Lie algebra $\mathfrak{D}$ contains the images of the carma moulds obtained for multiple zeta values (Definition B.61) under the map θ^D_{BIMU} (Proposition 5.29),

$$\theta^D_{\mathrm{BIMU}}(\mathfrak{C}) \subset \mathfrak{D}.$$

Not all relations in $\mathfrak{F}^{(2)}$ produce non-trivial generators for $\mathfrak{D}$, for example, the Eisenstein relations given in (5.34.1) should lift to proper relations in $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$. More precisely, the following number of generators and relations in $\mathcal{D}$ is expected.

Conjecture 5.38. *([Kü19]) The Lie algebra $\mathfrak{D}$ is a free Lie algebra and the Hilbert-Poincare series of its universal enveloping algebra is given by*

$$H_{\mathcal{U}(\mathfrak{D})}(x,y) = \sum_{w,d\geq 0} \dim_{\mathbb{Q}} \mathcal{U}(\mathfrak{D})^{(w,d)} x^w y^d = \frac{1}{1 - a_4(x)y^4},$$

where $a_4(x) = \frac{1}{1-x^2} \sum_{k\geq 12} \dim(\mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z})))^2 x^k$.

Finally, we want to investigate the relations between the two Lie algebras $\mathfrak{F}$ and $\mathfrak{D}$. Similar to the case of the ekma moulds (5.34.1), one obtains for any carma mould $C \in \mathfrak{C}$

$$\delta^m \operatorname{ari}\left(\operatorname{gr}_D \xi \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \theta^D_{\mathrm{BIMU}}(C)\right) = 0, \qquad m \geq 0. \tag{5.38.1}$$

Conjecture 5.39. *([Kü19])*

(i) The two Lie algebras $\mathfrak{F}$ *and* $\mathfrak{D}$ *generate the whole associated depth-graded Lie algebra* $\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$.

(ii) There are no relations between $\mathfrak{F}$ *and* $\mathfrak{D}$ *expect for the ones given in* (5.38.1).

Theorem 5.40. *Assume that Conjectures 5.36, 5.38, 5.39, and B.64 hold. Then the Hilbert-Poincare series of the universal enveloping algebra of* $\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ *is given by*

$$H_{\mathcal{U}\left(\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\right)}(x,y) = \frac{1}{1 - a_1(x)y + a_2(x)y^2 - a_3(x)y^3 - a_4(x)y^4 + a_5(x)y^5},$$

where $a_i(x),\ i = 1, \ldots, 5$ *are defined in Conjecture 1.21.*
In particular, Conjecture 5.28 would hold.

Proof. By Conjecture 5.36 and 5.38, one has

$$H_{\mathcal{U}(\mathfrak{F})}(x,y) = \frac{1}{1 - a_1(x)y + a_2(x)y^2 - a_3(x)y^3}, \qquad H_{\mathcal{U}(\mathfrak{D})}(x,y) = \frac{1}{1 - a_4(x)y^4}.$$

The number of generators of $\mathfrak{C}$ in weight k is expected to be given by $\dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))$ (Conjecture B.64). Thus, the number of relations in (5.38.1) is given by $D(x)xS(x) = a_5(x)$ (as before, the term $D(x)$ counts the derivations) and evidently, the relations in (5.38.1) are generated in depth 5. Since we assume that there are no further relations between $\mathfrak{F}$ and $\mathfrak{D}$ and both together generate $\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}$ (Conjecture 5.39), we deduce

$$H_{\mathcal{U}\left(\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\right)}(x,y) = \frac{1}{1 - a_1(x)y + a_2(x)y^2 - a_3(x)y^3 - a_4(x)y^4 + a_5(x)y^5}.$$

By definition of the numbers $g_{w,d}$ (Lemma 4.70), we immediately deduce Conjecture 5.28,

$$\dim_{\mathbb{Q}} \operatorname{gr}^{(d)}_D \left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}\right)^{(w)} = g_{w,d}.$$

□

In particular, the expected structure of $\left(\operatorname{gr}_D \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}, \operatorname{ari}\right)$ is compatible with the depth-graded dimension conjecture 1.21 (ii) for the multiple q-zeta values.

5.3 Symmetries of bimoulds related to balanced multiple q-zeta values

To compare the two approaches to Lie algebras related to multiple q-zeta values (Section 4 and Subsections 5.1, 5.2), we have to explain some terminology. In Definition 2.66 and 2.67, we introduced q-symmetral and q-symmetril bimoulds. In order to obtain Lie algebra structures, we will consider these properties modulo products. In the following, we will work over some fixed commutative $\mathbb{Q}$-algebra R with unit. Moreover, we only consider bimoulds with polynomial or power series components. In particular, we will drop both indices in the notation in the following.

Definition 5.41. A bimould $A \in \mathrm{BARI}$ is called q-alternal if there is a $\mathbb{Q}$-linear map $\varphi_{ш} : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to R$ satisfying $\varphi_{ш}(u \,ш\, v) = 0$ for all $u, v \in \mathbb{Q}\langle\mathcal{B}\rangle^0 \backslash \mathbb{Q}\mathbf{1}$, such that for all $d \geq 1$

$$A_d\begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d \geq 1 \\ m_1,\dots,m_d \geq 0}} \varphi_{ш}(b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}) X_1^{k_1-1} Y_1^{m_1} \dots X_d^{k_d-1} Y_d^{m_d}.$$

In this case, we refer to the map $\varphi_{ш}$ as the coefficient map of A.

The space of all q-alternal bimoulds is denoted by $\mathrm{BARI}_{q\text{-al}}$.

From the definition, we obtain that a bimould $A \in \mathrm{BARI}$ is q-alternal with coefficient map $\varphi_{ш}$ if and only if for all $0 < n < d$

$$\varphi_{ш}\left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} ш\, \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix}\right) = 0. \tag{5.41.1}$$

Here $\rho_{\mathcal{B}}(\mathcal{W})$ denotes the generating series of words in $\mathbb{Q}\langle\mathcal{B}\rangle^0$ as introduced in (2.65.2).

Definition 5.42. A bimould $A \in \mathrm{BARI}$ is called q-alternil if there is a $\mathbb{Q}$-linear map $\varphi_{*_q} : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to R$ satisfying $\varphi_{*_q}(u *_q v) = 0$ for all $u, v \in \mathbb{Q}\langle\mathcal{B}\rangle^0 \backslash \mathbb{Q}\mathbf{1}$, such that for all $d \geq 1$

$$A_d\begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d \geq 1 \\ m_1,\dots,m_d \geq 0}} \varphi_{*_q}(b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d}) X_1^{k_1-1} Y_1^{m_1} \dots X_d^{k_d-1} Y_d^{m_d}.$$

As before, we will refer to φ_{*_q} as the coefficient map of A.

By $\mathrm{BARI}_{q\text{-il}}$ we denote the subspace of all q-alternil bimoulds.

A bimould $A \in \mathrm{BARI}$ is q-alternil with coefficient map φ_{*_q} if and only if for all $0 < n < d$

$$\varphi_{*_q}\left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} *_q \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix}\right) = 0. \tag{5.42.1}$$

As in the case of alternality and alternility (Proposition C.19), q-alternality can be seen as the associated depth-graded symmetry to q-alternility.

Proposition 5.43. *Let $r \geq 1$ and $A = (0, 0, \dots, 0, A_r, A_{r+1}, \dots) \in \mathrm{BARI}_{q\text{-il}}$. Then $\mathrm{gr}_D\, A = (0, 0, \dots, 0, A_r, 0, 0, \dots)$ is a q-alternal bimould.*

Proof. By Proposition A.78 the explicit formulas for q-alternality (5.41.1) and q-alternility (5.42.1) differ only by terms of lower depth, this directly implies the claim. In particular, $\mathrm{gr}_D\, A$ is a q-alternal and q-alternil bimould at the same time. □

Definition 5.44. We define the following subspaces of BARI,

$$\mathrm{BARI}_{\underline{q\text{-al}},\tau} = \left\{ A \in \mathrm{BARI} \;\middle|\; \begin{array}{l} \cdot\ A \text{ is q-alternal,} \\ \cdot\ A \text{ is } \tau\text{-invariant,} \\ \cdot\ A\binom{X_1}{Y_1} \text{ is even} \end{array} \right\},$$

$$\mathrm{BARI}_{\underline{q\text{-il}},\tau} = \left\{ A \in \mathrm{BARI} \;\middle|\; \begin{array}{l} \cdot\ A \text{ is q-alternil,} \\ \cdot\ A \text{ is } \tau\text{-invariant,} \\ \cdot\ A\binom{X_1}{Y_1} \text{ is even} \end{array} \right\}.$$

The elements in $\mathrm{BARI}_{\underline{q\text{-il}},\tau}$ also satisfy a condition related to the product $*_\tau$. More precisely, we will state a version of Proposition 2.71 modulo products.

Proposition 5.45. *Let $A \in \mathrm{BARI}_{\underline{q\text{-il}},\tau}$, and $\varphi_{*_q} : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to R$ be the coefficient map of A. Then we have for all $0 < n < d$*

$$\varphi_{*_q}\left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} *_\tau \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix}\right) = 0.$$

Proof. As obtained in the proof of Proposition 2.71, we have $*_\tau = \tau \circ *_q \circ (\tau, \tau)$. Thus, we obtain the claim from the τ-invariance and the q-alternility of A. ☐

We relate the spaces $\mathrm{BARI}_{\underline{q\text{-al}},\tau}$ and $\mathrm{BARI}_{\underline{q\text{-il}},\tau}$ to the known spaces $\mathrm{BARI}_{\underline{\mathrm{al}},\mathrm{swap}}$ and $\mathrm{BARI}_{\underline{\mathrm{il}},\mathrm{swap}}$ (introduced in Theorem 5.2, 5.22).

Theorem 5.46. *We have two vector space isomorphisms*

$$\#_Y : \mathrm{BARI}_{\underline{q\text{-al}},\tau} \to \mathrm{BARI}_{\underline{\mathrm{al}},\mathrm{swap}}, \qquad \#_Y : \mathrm{BARI}_{\underline{q\text{-il}},\tau} \to \mathrm{BARI}_{\underline{\mathrm{il}},\mathrm{swap}}.$$

Proof. The proof consists of the same arguments as the proof of Theorem 2.75, just set the products to be zero. Observe that $\#_Y$ is the identity in depth 1, thus the condition that the depth 1 component of each bimould is even is preserved. ☐

Definition 5.47. For a bimould $A \in \mathrm{BIMU}$, denote

$$A^{\#_X}\begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix} = A\begin{pmatrix} X_1 + \dots + X_d, X_2 + \dots + X_d, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix}.$$

Note that we have by definition $\#_X = \tau \circ \#_Y \circ \tau$.

Corollary 5.48. *We have two vector space isomorphisms*

$$\tau \circ \#_X : \mathrm{BARI}_{\underline{q\text{-al}},\tau} \to \mathrm{BARI}_{\underline{\mathrm{al}},\mathrm{swap}}, \qquad \tau \circ \#_X : \mathrm{BARI}_{\underline{q\text{-il}},\tau} \to \mathrm{BARI}_{\underline{\mathrm{il}},\mathrm{swap}}.$$

Proof. Since $\tau \circ \#_Y \circ \tau = \#_X$, any τ-invariant bimould $A \in \mathrm{BIMU}$ satisfies $\tau(A^{\#_X}) = \tau(A)^{\#_Y} = A^{\#_Y}$. Thus the claim is obtained from Theorem 5.46. ☐

5.4 Bimoulds and $\mathfrak{bm}_0$

We will associate to each element in the space $\mathfrak{bm}_0$ (Definition 4.24) a bimould in $\mathrm{BARI}^{\mathbb{Q},\mathrm{pol}}$ (the general procedure is explained in Subsection A.4). Since the space $\mathfrak{bm}_0$ can be described in terms of three different alphabets, there are three different possibilities for the association. Each one yields bimoulds with different symmetries, which we will elaborate in detail in the following. These studies were an important part of finding the explicit formula of the q-Ihara bracket (Subsection 3.2). We state all the obtained detailed results here for further reference.

The alphabet $\mathcal{B}$. We start with the most natural translation of the space $\mathfrak{bm}_0$ into bimoulds, this means we consider the alphabet $\mathcal{B}$.

Definition 5.49. Consider the $\mathbb{Q}$-linear map

$$\rho_{\mathcal{B}} : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q}[X_1, Y_1, X_2, Y_2, \ldots],$$
$$b_{k_1} b_0^{m_1} \ldots b_{k_d} b_0^{m_d} \mapsto X_1^{k_1-1} Y_1^{m_1} \ldots X_d^{k_d-1} Y_d^{m_d}.$$

Let $\left(\mathbb{Q}\langle\mathcal{B}\rangle^0\right)^{(d)}$ the homogeneous component of $\mathbb{Q}\langle\mathcal{B}\rangle^0$ of depth d and for each $f \in \mathbb{Q}\langle\mathcal{B}\rangle^0$ denote by $f^{(d)}$ the homogeneous component of f of depth d. Then to every $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ we associate a bimould $\rho_{\mathcal{B}}(f) = (\rho_{\mathcal{B}}(f)_d)_{d \geq 0} \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ by

$$\rho_{\mathcal{B}}(f)_d \begin{pmatrix} X_1, \ldots, X_d \\ Y_1, \ldots, Y_d \end{pmatrix} = \rho_{\mathcal{B}}\Big(\Pi_0(f)^{(d)}\Big), \quad d \geq 1.$$

Note that the map $(\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc}) \to (\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}, \mathrm{mu})$, $f \mapsto \rho_{\mathcal{B}}(f)$ is not an algebra morphism. This is only the case if we restrict to $\mathbb{Q}\langle\mathcal{B}\rangle^0$.

Theorem 5.50. *For every $f \in \mathfrak{bm}_0$, the bimould $\rho_{\mathcal{B}}(f)$ is q-alternil and τ-invariant. More precisely, there is a vector space isomorphism*

$$\mathfrak{bm}_0 \xrightarrow{\sim} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{q\text{-il}},\tau}, \; f \mapsto \rho_{\mathcal{B}}(f).$$

The space $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{q\text{-il}},\tau}$ is introduced in Definition 5.44.

Proof. First observe that there is an isomorphism $\Big(\mathbb{Q}\langle\mathcal{B}\rangle^0 \backslash \mathbb{Q}\mathbf{1}\Big) \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$, $f \mapsto \rho_{\mathcal{B}}(f)$. By definition a bimould $\rho_{\mathcal{B}}(f) \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ is q-alternil with coefficient map $\mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q}$, $w \mapsto (f \mid w)$ if and only if

$$(f \mid u *_q v) = 0 \quad \text{for all } u, v \in \mathbb{Q}\langle\mathcal{B}\rangle^0 \backslash \mathbb{Q}\mathbf{1}.$$

On the other hand, the duality given in Theorem 4.5 implies that an element $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ is primitive for Δ_q if and only if

$$(f \mid v *_q w) = 0 \quad \text{for all } v, w \in \mathbb{Q}\langle\mathcal{B}\rangle \backslash \mathbb{Q}\mathbf{1}.$$

Furthermore, if f is primitive for Δ_q, then f is contained in $\ker(\partial_0)$. In particular, by applying the map sec_q one can uniquely recover f from the projection $\Pi_0(f)$ (Proposition 4.47). This shows that there is an isomorphism $\mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle) \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{q\text{-il}}}$, $f \mapsto \rho_{\mathcal{B}}(f)$.

Next, observe that a bimould $\rho_{\mathcal{B}}(f) \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ is τ-invariant if and only if the coefficient satisfy

$$(f \mid w) = (f \mid \tau(w)) \quad \text{for all } w \in \mathbb{Q}\langle\mathcal{B}\rangle^0.$$

This follows immediately from the definition of τ (Definition 2.12) and the observation in (2.65.1). On the other hand $\tau : \mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q}\langle\mathcal{B}\rangle^0$ maps words onto words, thus $\tau\Big(\Pi_0(f)\Big) = \Pi_0(f)$ is equivalent to

$$(f \mid w) = (f \mid \tau(w)) \text{ for each word } w \in \mathbb{Q}\langle\mathcal{B}\rangle^0.$$

Therefore, an element $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ satisfies $\tau\Big(\Pi_0(f)\Big) = \Pi_0(f)$ if and only if the bimould $\rho_{\mathcal{B}}(f)$ is τ-invariant.

Finally, $f \in \mathfrak{bm}$ satisfies $(f \mid b_2) = (f \mid b_4) = (f \mid b_6) = 0$ if and only if $(f \mid b_k b_0^m) = 0$ for any $k+m$ even (Proposition 4.25). Equivalently, the coefficient of $X_1^{k-1}Y_1^m$ in $\rho_{\mathcal{B}}(f)_1$ vanishes for all $k+m$ even, which means that $\rho_{\mathcal{B}}(f)_1$ is even. Altogether, we have shown that $\mathfrak{bm}_0 \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{q\text{-il}},\tau}$, $f \mapsto \rho_{\mathcal{B}}(f)$ is an isomorphism. ☐

Corollary 5.51. *There is an isomorphism of vector spaces*

$$\mathfrak{bm}_0 \xrightarrow{\sim} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}} \quad f \mapsto \rho_{\mathcal{B}}(f)^{\#_Y}.$$

Proof. The isomorphism can be obtained immediately from Theorem 5.50 and Theorem 5.46. ☐

The pre-Lie multiplication s_f^q for the q-Ihara bracket (Definition 3.16) corresponds to the pre-Lie multiplication preuri (Definition 5.15) under the above isomorphism $\#_Y \circ \rho_{\mathcal{B}}$. To prove this, we restrict to the subspace $\mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)$ of primitive elements in $(\mathbb{Q}\langle\mathcal{B}\rangle, \mathrm{conc}, \Delta_q)$.

Theorem 5.52. *For $f, g \in \mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)$, one has*

$$\rho_{\mathcal{B}}\Big(s_f^q(g)\Big)^{\#_Y} = \mathrm{preuri}\Big(\rho_{\mathcal{B}}(f)^{\#_Y}, \rho_{\mathcal{B}}(g)^{\#_Y}\Big).$$

Proof. Define the auxiliary letters

$$D_{k,m} = \Big(-\mathrm{ad}(b_0)\Big)^m(b_k) = [\cdots[[b_k, \underbrace{b_0], b_0]\cdots, b_0]}_{m \text{ times}}), \quad k \geq 1, m \geq 0.$$

By rewriting the letters v_i in terms of the alphabet $\mathcal{B}$ in Proposition 4.32 (according to Definition 4.29), we see that any element in $\mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)$ is a $\mathbb{Q}$-linear combination of words in the letters $D_{k,m}$. Consider the $\mathbb{Q}$-linear map

$$\begin{aligned}\rho_{\mathcal{D}} &: \mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle) \to \mathbb{Q}[X_1, Y_1, X_2, Y_2, \ldots],\\ D_{k_1,m_1}\ldots D_{k_d,m_d} &\mapsto X_1^{k_1-1}Y_1^{m_1}\ldots X_d^{k_d-1}Y_d^{m_d}.\end{aligned}$$

Let $\mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)^{(d)}$ be the homogeneous subspace of $\mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)$ spanned by all words in the letters $D_{k,m}$ of depth d and for each $f \in \mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)$ denote by $f^{(d)}$ the homogeneous component of f of depth d. We associate to each $f \in \mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)$ the bimould $\rho_{\mathcal{D}}(f) = \big(\rho_{\mathcal{D}}(f)_d\big)_{d\geq 0} \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ by

$$\rho_{\mathcal{D}}(f)_d\begin{pmatrix}X_1, \ldots, X_d\\ Y_1, \ldots, Y_d\end{pmatrix} = \rho_{\mathcal{D}}\Big(f^{(d)}\Big), \quad d \geq 1.$$

For some word $w = D_{k_1,m_1}\ldots D_{k_d,m_d}$ and each $d \geq 1$ compute

$$\begin{aligned}\Pi_0(w) &= b_{k_1}b_0^{m_1}\Big(-\mathrm{ad}(b_0)\Big)^{m_2}(b_{k_2})\ldots\Big(-\mathrm{ad}(b_0)\Big)^{m_d}(b_{k_d})\\ &= \sum_{n_2=0}^{m_2}\cdots\sum_{n_d=0}^{m_d}\binom{m_2}{n_2}\cdots\binom{m_d}{n_d}(-1)^{n_2+\cdots+n_d}b_{k_1}b_0^{m_1+n_2}b_{k_2}b_0^{m_2-n_2+n_3}\ldots b_{k_d}b_0^{m_d-n_d}\end{aligned}$$

and thus

$$\rho_{\mathcal{B}}(w)\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} = \sum_{n_2=0}^{m_2}\cdots\sum_{n_d=0}^{m_d}\binom{m_2}{n_2}\cdots\binom{m_d}{n_d}(-1)^{n_2+\cdots+n_d}X_1^{k_1-1}\dots X_d^{k_d-1} \cdot Y_1^{m_1+n_2}Y_2^{m_2-n_2+n_3}\dots Y_d^{m_d-n_d}$$

$$= X_1^{k_1-1}\dots X_d^{k_d-1}Y_1^{m_1}(Y_2-Y_1)^{m_2}(Y_3-Y_2)^{m_3}\dots(Y_d-Y_{d-1})^{m_d}$$

$$= \rho_{\mathcal{D}}(w)\binom{X_1,\dots,X_d}{Y_1,Y_2-Y_1,Y_3-Y_2\dots,Y_{d-1}-Y_d}$$

We deduce $\rho_{\mathcal{B}}(w)^{\#_Y} = \rho_{\mathcal{D}}(w)$. Therefore, it is enough to show that

$$\rho_{\mathcal{D}}\Big(s_f^q(g)\Big) = \operatorname{preuri}\Big(\rho_{\mathcal{D}}(f),\rho_{\mathcal{D}}(g)\Big), \qquad f,g\in \operatorname{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle).$$

Since all maps are $\mathbb{Q}$-linear, we can assume that $f = D_{k_1,m_1}\dots D_{k_d,m_d},\ g = D_{l_1,n_1}\dots D_{l_e,n_e}$. By definition, we obtain

$$d_f^q(g) = \sum_{i=1}^{e}\sum_{k_1'=0}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\binom{k_1-1}{k_1'}\cdots\binom{k_d-1}{k_d'}(-1)^{k_1'+\cdots+k_d'}D_{l_1,n_1}\dots D_{l_{i-1},n_{i-1}} \cdot \Big(-\operatorname{ad}(b_0)\Big)^{n_i}\Big(\Big[D_{k_1-k_1',m_1}\dots b_{k_d-k_d',m_d}, D_{l_i+k_1'+\cdots+k_d',0}\Big]\Big)D_{l_{i+1}n_{i+1}}\dots D_{l_e,n_e}$$

$$+\sum_{r=1}^{k_1+\cdots+k_d-d}\sum_{i=1}^{e}\sum_{\substack{k_1'=0\\(k_1',\dots,k_d')\neq(0,\dots,0)}}^{k_1-1}\cdots\sum_{k_d'=0}^{k_d-1}\binom{k_1-1}{k_1'}\cdots\binom{k_d-1}{k_d'}(-1)^{r+k_1'+\cdots+k_d'}$$

$$\sum_{\substack{j_1+\cdots+j_{r+1}=k_1'+\cdots+k_d'+1\\ j_1,\dots,j_{r+1}\geq 1}} D_{l_1,n_1}\dots D_{l_{i-1},n_{i-1}}\Big(-\operatorname{ad}(b_0)\Big)^{n_i}\Big(D_{l_i+j_1-1,0}D_{j_2,0}\dots D_{j_r,0} \cdot\Big[D_{k_1-k_1',m_1}\dots D_{k_d-k_d',m_d}, D_{j_{r+1},0}\Big]\Big)D_{l_{i+1},n_{i+1}}\dots D_{l_e,n_e}.$$

On the other hand, observe that we have for $1\leq i\leq j\leq d$

$$(Y_i+\cdots+Y_j)\rho_{\mathcal{D}}(D_{k_1,m_1}\dots D_{k_d,m_d})\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}$$

$$=\sum_{s=i}^{j}X_1^{k_1}\dots X_d^{k_d-1}Y_1^{m_1}\dots Y_{s-1}^{m_{s-1}}Y_s^{m_s+1}Y_{s+1}^{m_{s+1}}\dots Y_d^{m_d}$$

$$=\rho_{\mathcal{D}}\Big(\sum_{s=i}^{j}D_{k_1,m_1}\dots D_{k_{s-1},m_{s-1}}D_{k_s,m_s+1}D_{k_{s+1},m_{s+1}}\dots D_{k_d,m_d}\Big)\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}$$

$$=\rho_{\mathcal{D}}\Big(D_{k_1,m_1}\dots D_{k_{i-1},m_{i-1}}\big(-\operatorname{ad}(b_0)\big)\big(D_{k_i,m_i}\dots D_{k_j,m_j}\big)D_{k_{j+1},m_{j+1}} \dots D_{k_d,m_d}\Big)\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d},$$

where the last step follows from the observation that $-\operatorname{ad}(b_0)$ acts as a derivation on the letters $D_{k,m}$. Iteratively we get for each $n\geq 1$

$$(Y_i+\cdots+Y_j)^n\rho_{\mathcal{D}}(D_{k_1,m_1}\dots D_{k_d,m_d})\binom{X_1,\dots,X_d}{Y_1,\dots,Y_d} \tag{5.52.1}$$

$$= \rho_{\mathcal{D}}\Big(D_{k_1,m_1} \dots D_{k_{i-1},m_{i-1}}\Big(-\operatorname{ad}(b_0)\Big)^n (D_{k_i,m_i} \dots D_{k_j,m_j}) D_{k_{j+1},m_{j+1}} \dots D_{k_d,m_d}\Big)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix}.$$

With (5.52.1) compute

$$\begin{aligned}
&\operatorname{arit}_{\rho_{\mathcal{D}}(f)}(\rho_{\mathcal{D}}(g))\begin{pmatrix} X_1,\dots,X_{d+e} \\ Y_1,\dots,Y_{d+e} \end{pmatrix} \\
&= \sum_{i=1}^{e} \rho_{\mathcal{D}}(g)\begin{pmatrix} X_1,\dots,X_{i-1},X_{i+d},X_{i+d+1},\dots,X_{d+e} \\ Y_1,\dots,Y_{i-1},Y_i+\dots+Y_{i+d},Y_{i+d+1},\dots,Y_{d+e} \end{pmatrix} \\
&\qquad \cdot \rho_{\mathcal{D}}(f)\begin{pmatrix} X_i - X_{i+d},\dots,X_{i+d-1}-X_{i+d} \\ Y_i,\dots,Y_{i+d-1} \end{pmatrix} \\
&\quad - \sum_{i=1}^{e} \rho_{\mathcal{D}}(g)\begin{pmatrix} X_1,\dots,X_{i-1},X_i,X_{i+d+1},\dots,X_{d+e} \\ Y_1,\dots,Y_{i-1},Y_i+\dots+Y_{i+d},Y_{i+d+1},\dots,Y_{d+e} \end{pmatrix} \\
&\qquad \cdot \rho_{\mathcal{D}}(f)\begin{pmatrix} X_{i+1} - X_i,\dots,X_{i+d}-X_i \\ Y_{i+1},\dots,Y_{i+d} \end{pmatrix} \\
&= \sum_{i=1}^{e} X_1^{l_1-1}\dots X_{i-1}^{l_{i-1}-1} X_{i+d+1}^{l_{i+1}}\dots X_{d+e}^{l_e} Y_1^{n_1}\dots Y_{i-1}^{n_{i-1}} (Y_i+\dots+Y_{i+d})^{n_i} Y_{i+d+1}^{n_{i+1}}\dots Y_{d+e}^{n_e} \\
&\quad \cdot \Big(X_{i+d}^{l_i}(X_i - X_{i+d})^{k_1-1}\dots(X_{i+d-1}-X_{i+d})^{k_d-1} Y_i^{m_1}\dots Y_{i+d-1}^{m_d} \\
&\qquad - X_i^{l_i}(X_{i+1}-X_i)^{k_1-1}\dots(X_{i+d}-X_i)^{k_d-1} Y_{i+1}^{m_1}\dots Y_{i+d}^{m_d}\Big) \\
&= \sum_{i=1}^{e} X_1^{l_1-1}\dots X_{i-1}^{l_{i-1}-1} X_{i+d+1}^{l_{i+1}}\dots X_{d+e}^{l_e} Y_1^{n_1}\dots Y_{i-1}^{n_{i-1}} (Y_i+\dots+Y_{i+d})^{n_i} Y_{i+d+1}^{n_{i+1}}\dots Y_{d+e}^{n_e} \\
&\quad \cdot \sum_{k_1'=0}^{k_1-1}\dots\sum_{k_d'=0}^{k_d-1}\binom{k_1-1}{k_1'}\dots\binom{k_d-1}{k_d'}(-1)^{k_1'+\dots+k_d'} \\
&\quad \cdot \Bigg(X_{i+d}^{l_i+k_1'+\dots+k_d'} X_i^{k_1-k_1'-1}\dots X_{i+d-1}^{k_d-k_d'-1} Y_i^{m_1}\dots Y_{i+d-1}^{m_d} \\
&\qquad - X_i^{l_i+k_1'+\dots+k_d'} X_{i+1}^{k_1-k_1'-1}\dots X_{i+d}^{k_d-k_d'-1} Y_{i+1}^{m_1}\dots Y_{i+d}^{m_d}\Bigg) \\
&= \rho_{\mathcal{D}}\Bigg(\sum_{i=1}^{e}\sum_{k_1'=0}^{k_1-1}\dots\sum_{k_d'=0}^{k_d-1}\binom{k_1-1}{k_1'}\dots\binom{k_d-1}{k_d'}(-1)^{k_1'+\dots+k_d'} D_{l_1,n_1}\dots D_{l_{i-1},n_{i-1}} \\
&\quad \cdot \Big(-\operatorname{ad}(b_0)\Big)^{n_i}\Big(\Big[D_{k_1-k_1',m_1}\dots D_{k_d-k_d',m_d}, D_{l_i+k_1'+\dots+k_d',0}\Big]\Big) D_{l_{i+1},n_{i+1}} \\
&\qquad \dots D_{l_e,n_e}\Bigg)\begin{pmatrix} X_1,\dots,X_{d+e} \\ Y_1,\dots,Y_{d+e} \end{pmatrix}.
\end{aligned}$$

Moreover, with (5.14.1) and (5.52.1) we obtain for $r \geq 1$

$$\operatorname{urit}_{\rho_{\mathcal{D}}(f)}(\rho_{\mathcal{D}}(g))^{(d,e,r)}\begin{pmatrix} X_1,\dots,X_{d+e+r} \\ Y_1,\dots,Y_{d+e+r} \end{pmatrix}$$

$$= \sum_{i=1}^{e} \rho_{\mathcal{D}}(g) \begin{pmatrix} X_1, \dots, X_{i-1}, X_i, X_{i+1+d+r}, \dots, X_{d+e+r} \\ Y_1, \dots, Y_{i-1}, Y_i + \dots + Y_{i+d+r}, Y_{i+1+d+r}, \dots, Y_{d+e+r} \end{pmatrix}$$

$$\cdot \Bigg[\sum_{\substack{0 \le s \le r-1 \\ \text{or} \\ s=d+r}} \prod_{\substack{0 \le k \le r-1,\ k \ne s \\ \text{or} \\ k=d+r,\ k\ne s}} \frac{1}{(X_{i+k} - X_{i+s})} \rho_{\mathcal{D}}(f) \begin{pmatrix} X_{i+r} - X_{i+s}, \dots, X_{i+d+r-1} - X_{i+s} \\ Y_{i+r}, \dots, Y_{i+d+r-1} \end{pmatrix}$$

$$- \sum_{s=0}^{r} \prod_{\substack{k=0 \\ k \ne s}}^{r} \frac{1}{(X_{i+k} - X_{i+s})} \rho_{\mathcal{D}}(f) \begin{pmatrix} X_{i+1+r} - X_{i+s}, \dots, X_{i+d+r} - X_{i+s} \\ Y_{i+1+r}, \dots, Y_{i+d+r} \end{pmatrix} \Bigg]$$

$$= \sum_{i=1}^{e} X_1^{l_1-1} \dots X_i^{l_i-1} X_{i+1+d+r}^{l_{i+1}-1} \dots X_{d+e+r}^{l_e-1} Y_1^{n_1} \dots Y_{i-1}^{n_{i-1}} (Y_i + \dots + Y_{i+d+r})^{n_i}$$

$$\cdot Y_{i+1+d+r}^{n_{i+1}} \dots Y_{d+e+r}^{n_e}$$

$$\cdot \Bigg[\sum_{\substack{k_1'=0 \\ (k_1',\dots,k_d') \ne (0,\dots,0)}}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \binom{k_1-1}{k_1'} \dots \binom{k_d-1}{k_d'} (-1)^{r+k_1'+\dots+k_d'} \sum_{j_1+\dots+j_{r+1} = k_1'+\dots+k_d'+1}$$

$$\cdot X_i^{j_1-1} X_{i+1}^{j_2-1} \dots X_{i+r-1}^{j_r-1} X_{i+r}^{k_1-k_1'-1} \dots X_{i+d+r-1}^{k_d-k_d'-1} X_{i+d+r}^{j_{r+1}-1} Y_{i+r}^{m_1} \dots Y_{i+d+r-1}^{m_d}$$

$$- \sum_{\substack{k_1'=0 \\ (k_1',\dots,k_d') \ne (0,\dots,0)}}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \binom{k_1-1}{k_1'} \dots \binom{k_d-1}{k_d'} (-1)^{r+k_1'+\dots+k_d'} \sum_{j_1+\dots+j_{r+1} = k_1'+\dots+k_d'+1}$$

$$\cdot X_i^{j_1-1} X_{i+1}^{j_2-1} \dots X_{i+r}^{j_{r+1}-1} X_{i+r+1}^{k_1-k_1'-1} \dots X_{i+d+r}^{k_d-k_d'-1} Y_{i+r+1}^{m_1} \dots Y_{i+d+r}^{m_d} \Bigg]$$

$$= \rho_{\mathcal{D}} \Bigg(\sum_{i=1}^{d} \sum_{\substack{k_1'=0 \\ (k_1',\dots,k_d') \ne (0,\dots,0)}}^{k_1-1} \cdots \sum_{k_d'=0}^{k_d-1} \binom{k_1-1}{k_1'} \dots \binom{k_d-1}{k_d'} (-1)^{r+k_1'+\dots+k_d'} \sum_{j_1+\dots+j_{r+1} = k_1'+\dots+k_d'+1}$$

$$\cdot D_{l_1,n_1} \dots D_{l_{i-1},n_{i-1}} \Big(-\operatorname{ad}(b_0) \Big)^{n_i} \Big(D_{l_i+j_1-1,0} D_{j_2,0} \dots D_{j_r,0} \Big[D_{k_1-k_1',m_1}$$

$$\dots D_{k_d-k_d',m_d}, D_{j_{r+1},0} \Big] \Big) D_{l_{i+1},n_{i+1}} \dots D_{l_e,n_e} \Bigg) \begin{pmatrix} X_1, \dots, X_{d+e+r} \\ Y_1, \dots, Y_{d+e+r} \end{pmatrix}.$$

Since

$$\operatorname{urit}_{\rho_{\mathcal{D}}(f)}(\rho_{\mathcal{D}}(g)) \begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} = \operatorname{arit}_{\rho_{\mathcal{D}}(f)}(\rho_{\mathcal{D}}(g))$$
$$+ \operatorname{urit}_{\rho_{\mathcal{D}}(f)}(\rho_{\mathcal{D}}(g))^{d,e,n-d-e} \begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix},$$

comparing the computed formulas yields

$$\rho_{\mathcal{D}}\Big(d_f^q(g)\Big) = \operatorname{urit}_{\rho_{\mathcal{D}}(f)} \Big(\rho_{\mathcal{D}}(g)\Big).$$

Moreover, the map $(\operatorname{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle), \operatorname{conc}) \to (\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}, \operatorname{mu})$, $f \mapsto \rho_{\mathcal{D}}(f)$ is an algebra morphism. For two elements $f, g \in \operatorname{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)$ the homogeneous component of fg of depth d (with respect to the letters $D_{k,m}$) is given by

$$(fg)^{(d)} = \sum_{i=1}^{d-1} f^{(i)} g^{(d-i)}.$$

Thus, we obtain $\rho_{\mathcal{D}}(fg)_1 = \mathrm{mu}(\rho_{\mathcal{D}}(f), \rho_{\mathcal{D}}(g))_1 = 0$ and for each $d \geq 2$

$$\rho_{\mathcal{D}}(fg)\binom{X_1, \dots, X_d}{Y_1, \dots, Y_d} = \sum_{i=1}^{d-1} \rho_{\mathcal{D}}(f)\binom{X_1, \dots, X_i}{Y_1, \dots, Y_i} \rho_{\mathcal{D}}(g)\binom{X_{i+1}, \dots, X_d}{Y_{i+1}, \dots, Y_d}$$
$$= \mathrm{mu}\left(\rho_{\mathcal{D}}(f), \rho_{\mathcal{D}}(g)\right)\binom{X_1, \dots, X_d}{Y_1, \dots, Y_d}.$$

We deduce that for all $f, g \in \mathrm{Prim}(\mathbb{Q}\langle\mathcal{B}\rangle)$

$$\rho_{\mathcal{D}}\left(s_f^q(g)\right) = \rho_{\mathcal{D}}\left(d_f^q(g)\right) + \rho_{\mathcal{D}}(gf) = \mathrm{urit}_{\rho_{\mathcal{D}}(f)}\left(\rho_{\mathcal{D}}(g)\right) + \mathrm{mu}\left(\rho_{\mathcal{D}}(g), \rho_{\mathcal{D}}(f)\right)$$
$$= \mathrm{preuri}\left(\rho_{\mathcal{D}}(f), \rho_{\mathcal{D}}(g)\right).$$

□

Due to Theorem 5.52 and Corollary 5.51, Conjectures 5.16, 5.19, and 4.52 can be summarized as follows.

Conjecture 5.53. *There is a Lie algebra isomorphism*

$$\left(\mathfrak{bm}_0, \{-,-\}_q\right) \xrightarrow{\sim} \left(\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{il}},\mathrm{swap}}, \mathrm{uri}\right),\ f \mapsto \rho_{\mathcal{B}}(f)^{\#_Y}.$$

The alphabet $\mathcal{V}$. Consider the alphabet $\mathcal{V}$ and recall that by Corollary 4.33, the space $\mathfrak{bm}_0$ is contained in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$.

Set $\mathrm{dep}(v_0) = 0$ and $\mathrm{dep}(v_k) = 1$ for $k \geq 1$, this defines an ascending filtration on $\mathbb{Q}\langle\mathcal{V}\rangle$. Note that the notions of depth for $\mathbb{Q}\langle\mathcal{B}\rangle$ and $\mathbb{Q}\langle\mathcal{V}\rangle$ induce the same filtration under the identification given in Definition 4.29. Let $\mathbb{Q}\langle\mathcal{V}\rangle^0$ be the subalgebra of $\mathbb{Q}\langle\mathcal{V}\rangle$ generated by all words, which do not start in v_0. Moreover, we denote by $(\mathbb{Q}\langle\mathcal{V}\rangle^0)^{(d)}$ the homogeneous component of $\mathbb{Q}\langle\mathcal{V}\rangle^0$ of depth d.

Definition 5.54. Consider the $\mathbb{Q}$-linear map

$$\rho_{\mathcal{V}}: \mathbb{Q}\langle\mathcal{V}\rangle^0 \to \mathbb{Q}[X_1, Y_1, X_2, Y_2, \dots],$$
$$v_{k_1}v_0^{m_1}\dots v_{k_d}v_0^{m_d} \mapsto X_1^{k_1-1}Y_1^{m_1}\dots X_d^{k_d-1}Y_d^{m_d}.$$

To each $f \in \mathbb{Q}\langle\mathcal{V}\rangle$, associate a bimould $\rho_{\mathcal{V}}(f) = \left(\rho_{\mathcal{V}}(f)_d\right)_{d\geq 0} \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ by

$$\rho_{\mathcal{V}}(f)_d\binom{X_1, \dots, X_d}{Y_1, \dots, Y_d} = \rho_{\mathcal{V}}\left(\Pi_0(f)^{(d)}\right), \qquad d \geq 1,$$

where $f^{(d)} \in (\mathbb{Q}\langle\mathcal{V}\rangle^0)^{(d)}$ denotes the homogeneous component of f of depth d.

Note that the map $(\mathbb{Q}\langle\mathcal{V}\rangle, \mathrm{conc}) \to (\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}, \mathrm{mu}),\ f \mapsto \rho_{\mathcal{V}}(f)$ is not an algebra morphism.

Proposition 5.55. *For an element $f \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$ the bimould $\rho_{\mathcal{V}}(f)$ is q-alternal. More precisely, there is a vector space isomorphism*

$$\left\{f \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle \;\middle|\; (f \mid v_0) = 0\right\} \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{q\text{-al}},\ f \mapsto \rho_{\mathcal{V}}(f).$$

Proof. There is an isomorphism $\left(\mathbb{Q}\langle\mathcal{V}\rangle^0\backslash\mathbb{Q}\mathbf{1}\right) \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}},\ f \mapsto \rho_{\mathcal{V}}(f)$. By definition a bimould $\rho_{\mathcal{V}}(f) \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ is q-alternal with coefficient map

$$\mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q},\ b_{k_1}b_0^{m_1}\dots b_{k_d}b_0^{m_d} \mapsto (f \mid v_{k_1}v_0^{m_1}\dots v_{k_d}v_0^{m_d})$$

if and only if

$$(f \mid u \sqcup\!\sqcup\, v) = 0 \text{ for all } v, w \in \mathbb{Q}\langle\mathcal{V}\rangle^0\backslash\mathbb{Q}\mathbf{1}.$$

On the other hand, an element $f \in \mathbb{Q}\langle\mathcal{V}\rangle$ is contained in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$ if and only if it is primitive for the shuffle coproduct $\Delta_{\sqcup\!\sqcup} : \mathbb{Q}\langle\mathcal{V}\rangle \to \mathbb{Q}\langle\mathcal{V}\rangle \otimes \mathbb{Q}\langle\mathcal{V}\rangle$ (Corollary A.40). By duality (Example A.62) being primitive for $\Delta_{\sqcup\!\sqcup}$ is equivalent to

$$(f \mid v \sqcup\!\sqcup\, w) = 0 \text{ for all } v, w \in \mathbb{Q}\langle\mathcal{V}\rangle\backslash\mathbb{Q}\mathbf{1}.$$

In particular, for $f \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$ the bimould $\rho_{\mathcal{V}}(f)$ is q-alternal. Moreover, we have by Proposition 4.45 and Proposition 4.47 (i)

$$\left\{f \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle \;\middle|\; (f \mid v_0) = 0\right\} = \ker(\partial_0).$$

Thus the map $\sec_q$ associates to every element in $\mathbb{Q}\langle V\rangle^0$ a unique element in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$ with vanishing coefficient at v_0. Thus, the isomorphism $\left(\mathbb{Q}\langle\mathcal{V}\rangle^0\backslash\mathbb{Q}\mathbf{1}\right) \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}},\ f \mapsto \rho_{\mathcal{V}}(f)$ restricts to an isomorphism from $\{f \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle \mid (f \mid v_0) = 0\}$ to $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{q\text{-al}}$. □

Let $f \in \mathbb{Q}\langle\mathcal{V}\rangle$ and r be the smallest number, such that f has a non-trivial component of depth r. Then by definition of the alphabet $\mathcal{V}$ (Definition 4.29), the following holds

$$\rho_{\mathcal{V}}(f)\begin{pmatrix} X_1, \dots, X_r \\ Y_1, \dots, Y_r \end{pmatrix} = \rho_{\mathcal{B}}(f)\begin{pmatrix} X_1, \dots, X_r \\ Y_1, \dots, Y_r \end{pmatrix}.$$

So by Theorem 5.50 the component $\rho_{\mathcal{V}}(f)_r$ is τ-invariant for $f \in \mathfrak{bm}_0$. We want to investigate the τ-invariance of some f in terms of the bimould $\rho_{\mathcal{V}}(f)$. Therefore, we will explain the translation of the alphabet $\mathcal{V}$ into the alphabet $\mathcal{B}$ (Definition 4.29) in terms of bimoulds.

Definition 5.56. Let $A \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ be a bimould. For $1 \le i \le j \le d$, we define

$$A\begin{pmatrix} X_1, \dots, X_{i-1}, [X_\bullet]_i^j, X_{j+1}, \dots, X_d \\ Y_1, \dots, Y_{i-1}, Y_j, Y_{j+1}, \dots, Y_d \end{pmatrix} = \\ \frac{(-1)^{j-i}}{j-i+1}\sum_{s=i}^{j}\prod_{\substack{k=i \\ k\neq s}}^{j}(Y_s - Y_k)^{-1} A\begin{pmatrix} X_1, \dots, X_{i-1}, X_s, X_{j+1}, \dots, X_d \\ Y_1, \dots, Y_{i-1}, Y_i, Y_{j+1}, \dots, Y_d \end{pmatrix}$$

and let $\mathrm{t}_{\mathcal{V},\mathcal{B}}(A)$ be the bimould given by

$$\mathrm{t}_{\mathcal{V},\mathcal{B}}(A)\begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix} = \sum_{r=1}^{d}\sum_{0<j_1<\dots<j_r=d} A\begin{pmatrix} [X_\bullet]_1^{j_1}, [X_\bullet]_{j_1+1}^{j_2}, \dots, [X_\bullet]_{j_{r-1}+1}^{j_r} \\ Y_{j_1}, Y_{j_2}, \dots, Y_{j_r} \end{pmatrix}$$

Extend the definition of the operators $[-]_i^j$ by distributivity, to evaluate several of them at the same time.

We call a bimould $A \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ quasi τ-invariant if the bimould $\mathrm{t}_{\mathcal{V},\mathcal{B}}(A)$ is τ-invariant.

Lemma 5.57. *The following equality of bimoulds holds for each* $f \in \mathbb{Q}\langle\mathcal{V}\rangle = \mathbb{Q}\langle\mathcal{B}\rangle$

$$\Big(\mathrm{t}_{\mathcal{V},\mathcal{B}} \circ \rho_{\mathcal{V}}\Big)(f) = \rho_{\mathcal{B}}(f).$$

Proof. Let $w = v_k v_0^m$. Then the component $w^{(d)} \in \mathbb{Q}\langle\mathcal{B}\rangle^0$ of depth d is given by (Definition 4.29)

$$w^{(d)} = \frac{(-1)^{d-1}}{d} \sum_{\substack{j_1+\dots+j_d=k \\ j_1,\dots,j_d \geq 1}} b_{j_1} \dots b_{j_d} b_0^m$$

and thus we deduce with (5.14.1)

$$\begin{aligned}
\rho_{\mathcal{B}}(w)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} &= \frac{(-1)^{d-1}}{d} \sum_{\substack{j_1+\dots+j_d=k \\ j_1,\dots,j_d \geq 1}} X_1^{j_1-1} \dots X_d^{j_d-1} Y_d^m \\
&= \frac{(-1)^{d-1}}{d} \sum_{s=1}^{d} \prod_{\substack{k=1 \\ k\neq s}}^{d} (X_s - X_k)^{-1} X_s^{k-1} Y_d^m \\
&= \frac{(-1)^{d-1}}{d} \sum_{s=1}^{d} \prod_{\substack{k=1 \\ k\neq s}}^{d} (X_s - X_k)^{-1} \rho_{\mathcal{V}}(w)\begin{pmatrix} X_s \\ Y_d \end{pmatrix} \\
&= \rho_{\mathcal{V}}(w)\begin{pmatrix} [X_\bullet]_1^d \\ Y_d \end{pmatrix} \\
&= \big(\mathrm{t}_{\mathcal{V},\mathcal{B}} \circ \rho_{\mathcal{V}}\big)(w)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix}
\end{aligned}$$

Thus, we have for any word $w = v_{k_1} v_0^{m_1} \dots v_{k_r} v_0^{m_r}$ and $d \geq r$ that

$$\begin{aligned}
\rho_{\mathcal{B}}(w)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} &= \sum_{0<j_1<\dots<j_r=d} \rho_{\mathcal{V}}(w)\begin{pmatrix} [X_\bullet]_1^{j_1}, [X_\bullet]_{j_1+1}^{j_2}, \dots, [X_\bullet]_{j_{r-1}+1}^{j_r} \\ Y_{j_1}, Y_{j_2}, \dots, Y_{j_r} \end{pmatrix} \\
&= \big(\mathrm{t}_{\mathcal{V},\mathcal{B}} \circ \rho_{\mathcal{V}}\big)(w)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix}.
\end{aligned}$$

Extending the arguments by linearity to all elements in $\mathbb{Q}\langle\mathcal{V}\rangle^0$, we obtain the claim. ☐

Definition 5.58. Define the following subspace of $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$

$$\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{q}\text{-al},\text{quasi-}\tau} = \left\{ A \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}} \;\middle|\; \begin{array}{l} \cdot\ A \text{ is q-alternal,} \\ \cdot\ A \text{ is quasi } \tau\text{-invariant,} \\ \cdot\ A\binom{X_1}{Y_1} \text{ is even} \end{array} \right\}.$$

Theorem 5.59. *There is an isomorphism of vector spaces*

$$\mathfrak{bm}_0 \xrightarrow{\sim} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{q}\text{-al},quasi\text{-}\tau},\ f \mapsto \rho_{\mathcal{V}}(f).$$

Proof. By Proposition 5.55 we have a vector space isomorphism

$$\Big\{ f \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle \;\Big|\; (f \mid v_0) = 0 \Big\} \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{q\text{-al}},\ f \mapsto \rho_{\mathcal{V}}(f).$$

By Proposition 4.32 an element $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ lies in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle$ is and only if f is primitive for Δ_q. Thus $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ satisfies the defining conditions (i) and (ii) of $\mathfrak{bm}_0$ (Definition 4.24) if and only if $\rho_{\mathcal{V}}(f)$ is contained in $\mathrm{BARI}_{q\text{-al}}^{\mathrm{pol},\mathbb{Q}}$. Moreover, by Theorem 5.50 and Lemma 5.57, an element $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ satisfies $\tau(\Pi_0(f)) = \Pi_0(f)$ if and only if $\mathrm{t}_{\mathcal{V},\mathcal{B}} \circ \rho_{\mathcal{V}}(f)$ is τ-invariant. By definition, this is equivalent to $\rho_{\mathcal{V}}(f)$ being quasi τ-invariant. Finally, by Proposition 4.25 an element $f \in \mathfrak{bm}$ satisfies $(f \mid b_2) = (f \mid b_4) = (f \mid b_6) = 0$ if and only if we have $(f \mid b_k b_0^m) = 0$ for all $k+m$ even. By definition of the alphabet $\mathcal{V}$, this is equivalent to $(f \mid v_k v_0^m) = 0$ for all $k+m$ even, which means $\rho_{\mathcal{V}}(f)_1$ must be even. □

The alphabet $\mathcal{C}^{\mathrm{bi}}$. Finally, we consider the alphabet $\mathcal{C}^{\mathrm{bi}}$. Recall that by Theorem 4.51 the space $\mathfrak{bm}_0$ can be purely described in the alphabet $\mathcal{C}^{\mathrm{bi}}$,

$$\mathfrak{bm}_0 \simeq \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{C}^{\mathrm{bi}}\rangle \cap \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle^{\underline{\tau}}.$$

Set $\mathrm{dep}(C_{k,m}) = 1$, this defines an ascending depth filtration on $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$. Denote by $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle^{(d)}$ the homogeneous subspace of depth d. The notions of depth for $\mathbb{Q}\langle\mathcal{B}\rangle$, $\mathbb{Q}\langle\mathcal{V}\rangle$, and $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$ induce all the same filtration under the identifications given in Definition 4.29, 4.44.

Definition 5.60. Consider the $\mathbb{Q}$-linear map

$$\begin{aligned}\rho_{\mathcal{C}^{\mathrm{bi}}} : \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle &\to \mathbb{Q}[X_1, Y_1, X_2, Y_2, \ldots],\\ C_{k_1,m_1}\ldots C_{k_d,m_d} &\mapsto X_1^{k_1-1}Y_1^{m_1}\ldots X_d^{k_d-1}Y_d^{m_d}.\end{aligned}$$

To every $f \in \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$ associate the bimould $\rho_{\mathcal{C}^{\mathrm{bi}}}(f) = \left(\rho_{\mathcal{C}^{\mathrm{bi}}}(f)_d\right)_{d\geq 0} \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ by

$$\rho_{\mathcal{C}^{\mathrm{bi}}}(f)_d\begin{pmatrix}X_1,\ldots,X_d\\ Y_1,\ldots,Y_d\end{pmatrix} = \rho_{\mathcal{C}^{\mathrm{bi}}}(f^{(d)}), \qquad d\geq 1,$$

where $f^{(d)} \in \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle^{(d)}$ denotes the homogeneous component of f of depth d.

Lemma 5.61. *The map* $(\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle\backslash\mathbb{Q}\mathbf{1}, \mathrm{conc}) \to (\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}, \mathrm{mu})$, $f \mapsto \rho_{\mathcal{C}^{\mathrm{bi}}}(f)$ *is an algebra morphism.*

Proof. For two elements $f, g \in \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle\backslash\mathbb{Q}\mathbf{1}$, the component of depth d of the product fg is given by

$$(fg)^{(d)} = \sum_{i=1}^{d-1} f^{(i)}g^{(d-i)}.$$

Thus we deduce for each $d \geq 2$ that

$$\begin{aligned}\rho_{\mathcal{C}^{\mathrm{bi}}}(fg)\begin{pmatrix}X_1,\ldots,X_d\\ Y_1,\ldots,Y_d\end{pmatrix} &= \sum_{i=1}^{d-1}\rho_{\mathcal{C}^{\mathrm{bi}}}(f)\begin{pmatrix}X_1,\ldots,X_i\\ Y_1,\ldots,Y_i\end{pmatrix}\rho_{\mathcal{C}^{\mathrm{bi}}}(g)\begin{pmatrix}X_{i+1},\ldots,X_d\\ Y_{i+1},\ldots,Y_d\end{pmatrix}\\ &= \mathrm{mu}(\rho_{\mathcal{C}^{\mathrm{bi}}}(f), \rho_{\mathcal{C}^{\mathrm{bi}}}(g))\begin{pmatrix}X_1,\ldots,X_d\\ Y_1,\ldots,Y_d\end{pmatrix}\end{aligned}$$

and moreover $\rho_{\mathcal{C}^{\mathrm{bi}}}(fg)_1 = \mathrm{mu}(\rho_{\mathcal{C}^{\mathrm{bi}}}(f), \rho_{\mathcal{C}^{\mathrm{bi}}}(g))_1 = 0$. □

Lemma 5.62. *For* $f \in \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$, *one has*

$$\rho_{\mathcal{C}^{\mathrm{bi}}}(f)\begin{pmatrix}X_1,\ldots,X_d\\ Y_1,\ldots,Y_d\end{pmatrix} = (\rho_{\mathcal{V}}(f))^{\#_Y}\begin{pmatrix}X_1,\ldots,X_d\\ Y_1,\ldots,Y_d\end{pmatrix}.$$

Proof. It is enough to proof the equality for words in $\mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$, thus let $w = C_{k_1,m_1}\dots C_{k_d,m_d}$. Then we obtain

$$\begin{aligned}\Pi_0(w) &= v_{k_1}v_0^{m_1}\Big(-\operatorname{ad}(v_0)\Big)^{m_2}(v_{k_2})\dots\Big(-\operatorname{ad}(v_0)\Big)^{m_d}(v_d)\\ &= \sum_{n_2=0}^{m_2}\cdots\sum_{n_d=0}^{m_d}\binom{m_2}{n_2}\cdots\binom{m_d}{n_d}(-1)^{n_2+\dots+n_d}v_{k_1}v_0^{m_1+n_2}v_{k_2}v_0^{m_2-n_2+n_3}\dots v_{k_d}v_0^{m_d-n_d}\end{aligned}$$

and thus

$$\begin{aligned}\rho_{\mathcal{V}}(f)\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix} &= \sum_{n_2=0}^{m_2}\cdots\sum_{n_d=0}^{m_d}\binom{m_2}{n_2}\cdots\binom{m_d}{n_d}(-1)^{n_2+\dots+n_d}X_1^{k_1-1}\dots X_d^{k_d-1}\\ &\qquad\qquad\cdot Y_1^{m_1+n_2}Y_2^{m_2-n_2+n_3}\dots Y_d^{m_d-n_d}\\ &= X_1^{k_1-1}\dots X_d^{k_d-1}Y_1^{m_1}(Y_2-Y_1)^{m_2}\dots(Y_d-Y_{d-1})^{m_d}\\ &= \rho_{\mathcal{C}^{\mathrm{bi}}}(w)\begin{pmatrix}X_1,\dots,X_d\\Y_1,Y_2-Y_1,\dots,Y_d-Y_{d-1}\end{pmatrix}\\ &= \rho_{\mathcal{C}^{\mathrm{bi}}}(w)^{\#_Y^{-1}}\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}.\end{aligned}$$

□

Proposition 5.63. *For $f \in \operatorname{Lie}_{\mathbb{Q}}\langle\mathcal{C}^{\mathrm{bi}}\rangle$, the bimould $\rho_{\mathcal{C}^{\mathrm{bi}}}(f)$ is alternal. More precisely, there is a vector space isomorphism*

$$\operatorname{Lie}_{\mathbb{Q}}\langle\mathcal{C}^{\mathrm{bi}}\rangle \xrightarrow{\sim} \mathrm{BARI}_{\mathrm{al}}^{\mathrm{pol},\mathbb{Q}},\ \ f\mapsto \rho_{\mathcal{C}^{\mathrm{bi}}}(f).$$

Proof. By Lazard elimination (Proposition 4.45), we can identify

$$\Big\{f\in \operatorname{Lie}_{\mathbb{Q}}\langle\mathcal{V}\rangle \;\Big|\; (f\mid v_0)=0\Big\} = \operatorname{Lie}_{\mathbb{Q}}\langle\mathcal{C}^{\mathrm{bi}}\rangle.$$

Thus, by Proposition 5.55 there is an isomorphism

$$\operatorname{Lie}_{\mathbb{Q}}\langle\mathcal{C}^{\mathrm{bi}}\rangle \to \mathrm{BARI}_{q\text{-al}}^{\mathrm{pol},\mathbb{Q}},\ \ f\mapsto \rho_{\mathcal{V}}(f).$$

Theorem 5.46 shows that $\#_Y$ induces an isomorphism

$$\#_Y : \mathrm{BARI}_{q\text{-al}}^{\mathrm{pol},\mathbb{Q}} \to \mathrm{BARI}_{\mathrm{al}}^{\mathrm{pol},\mathbb{Q}}.$$

Thus we deduce the claim from Lemma 5.62. □

Recall that $\#_Y$ maps a τ-invariant bimould to a swap invariant bimould (Theorem 5.46). Thus, by Lemma 5.62 we have for a τ-invariant element $f \in \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$ that the component of $\rho_{\mathcal{C}^{\mathrm{bi}}}(f)$ of lowest non-trivial depth is swap invariant. We want to investigate, what kind of relation the τ-invariance of some $f \in \mathbb{Q}\langle\mathcal{C}^{\mathrm{bi}}\rangle$ induces on the bimould $\rho_{\mathcal{C}^{\mathrm{bi}}}(f)$ in arbitrary depths.

Definition 5.64. For a bimould $A \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ define $\mathrm{t}_{\mathcal{C}^{\mathrm{bi}},\mathcal{B}}(A)$ by

$$\begin{aligned}&\mathrm{t}_{\mathcal{C}^{\mathrm{bi}},\mathcal{B}}(A)\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix}\\ &\quad=\sum_{r=1}^{d}\sum_{0<j_1<\dots<j_r=d}A\begin{pmatrix}[X_\bullet]_1^{j_1},[X_\bullet]_{j_1+1}^{j_2},\dots,[X_\bullet]_{j_{r-1}+1}^{j_r}\\Y_1+\dots+Y_{j_1},Y_{j_1+1}+\dots+Y_{j_2},\dots,Y_{j_{r-1}+1}+\dots+Y_{j_r}\end{pmatrix}.\end{aligned}$$

where the operator $[-]_i^j$ is given in Definition 5.56.

We say that a bimould $A \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ is q-swap invariant if the bimould $\mathrm{t}_{\mathcal{C}^{\mathrm{bi}},\mathcal{B}}$ is swap invariant.

Lemma 5.65. *The following equality of bimoulds holds for* $f \in \mathbb{Q}\langle \mathcal{C}^{\mathrm{bi}} \rangle \subset \mathbb{Q}\langle \mathcal{B} \rangle$

$$\Big(\mathrm{t}_{\mathcal{C}^{\mathrm{bi}},\mathcal{B}} \circ \rho_{\mathcal{C}^{\mathrm{bi}}} \Big)(f) = \rho_{\mathcal{B}}(f)^{\#_Y}.$$

Proof. For a bimould $A \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$, compute

$$\begin{aligned}
&\mathrm{t}_{\mathcal{V},\mathcal{B}} \left(A^{\#_Y^{-1}} \right)^{\#_Y} \begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix} = \mathrm{t}_{\mathcal{V},\mathcal{B}} \left(A^{\#_Y^{-1}} \right) \begin{pmatrix} X_1, \dots, X_d \\ Y_1, Y_1 + Y_2, \dots, Y_1 + \dots + Y_d \end{pmatrix} \\
&= \sum_{r=1}^{d} \sum_{0 < j_1 < \dots < j_r = d} A^{\#_Y^{-1}} \begin{pmatrix} [X_\bullet]_1^{j_1}, [X_\bullet]_{j_1+1}^{j_2}, \dots, [X_\bullet]_{j_{r-1}+1}^{j_r} \\ Y_1 + \dots + Y_{j_1}, Y_1 + \dots + Y_{j_2}, \dots, Y_1 + \dots + Y_{j_r} \end{pmatrix} \\
&= \sum_{r=1}^{d} \sum_{0 < j_1 < \dots < j_r = d} A \begin{pmatrix} [X_\bullet]_1^{j_1}, [X_\bullet]_{j_1+1}^{j_2}, \dots, [X_\bullet]_{j_{r-1}+1}^{j_r} \\ Y_1 + \dots + Y_{j_1}, Y_{j_1+1} + \dots + Y_{j_2}, \dots, Y_{j_{r-1}+1} + \dots + Y_{j_r} \end{pmatrix} \\
&= \mathrm{t}_{\mathcal{C}^{\mathrm{bi}},\mathcal{B}}(A) \begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix}.
\end{aligned}$$

Thus, we get

$$\mathrm{t}_{\mathcal{C}^{\mathrm{bi}},\mathcal{B}} \circ \rho_{\mathcal{C}^{\mathrm{bi}}} = \#_Y \circ \mathrm{t}_{\mathcal{V},\mathcal{B}} \circ \#_Y^{-1} \circ \rho_{\mathcal{C}^{\mathrm{bi}}} = \#_Y \circ \mathrm{t}_{\mathcal{V},\mathcal{B}} \circ \rho_{\mathcal{V}} = \#_Y \circ \rho_{\mathcal{B}},$$

where the second equality follows from Lemma 5.62 and the third equality from Lemma 5.57. ☐

Definition 5.66. Define the following subspace of $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$

$$\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},q\text{-swap}} = \left\{ A \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}} \;\middle|\; \begin{array}{l} \cdot\ A \text{ is alternal,} \\ \cdot\ A \text{ q-swap invariant,} \\ \cdot\ A\binom{X_1}{Y_1} \text{ is even} \end{array} \right\}.$$

Theorem 5.67. *There is a vector space isomorphism*

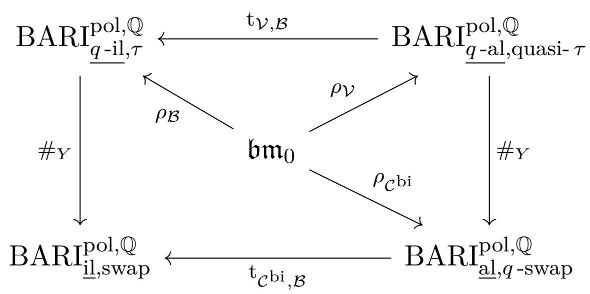
$$\mathfrak{bm}_0 \xrightarrow{\sim} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},q\text{-swap}}, \;\; f \mapsto \rho_{\mathcal{C}^{\mathrm{bi}}}(f).$$

Proof. By Proposition 5.63, there is a vector space isomorphism

$$\mathrm{Lie}_{\mathbb{Q}}\langle \mathcal{C}^{\mathrm{bi}} \rangle \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\mathrm{al}}, \;\; f \mapsto \rho_{\mathcal{C}^{\mathrm{bi}}}(f).$$

Furthermore, one has $f \in \mathbb{Q}\langle \mathcal{C}^{\mathrm{bi}} \rangle^{\underline{\tau}}$ if and only if $\tau(\Pi_0(f)) = \Pi_0(f)$ and $(f \mid C_{k,0}) = 0$ for $k = 2, 4, 6$ (Definition 4.50). By Corollary 5.51 the first condition is equivalent to $\rho_{\mathcal{B}}(f)^{\#_Y}$ being swap invariant. By Lemma 5.65 this is equivalent to $(\mathrm{t}_{\mathcal{C}^{\mathrm{bi}},\mathcal{B}} \circ \rho_{\mathcal{C}^{\mathrm{bi}}})(f)$ being swap invariant, so by definition that $\rho_{\mathcal{C}^{\mathrm{bi}}}$ is q-swap invariant. Finally, we have $(f \mid C_{k,0}) = 0$ for $k = 2, 4, 6$ if and only if $(f \mid C_{k,m}) = 0$ for all $k + m$ even (cf Proposition 4.25), which is by definition of $\rho_{\mathcal{C}^{\mathrm{bi}}}(f)$ equivalent to $\rho_{\mathcal{C}^{\mathrm{bi}}}(f)_1$ being even. From the description of the space $\mathfrak{bm}_0$ purely in the alphabet $\mathcal{C}^{\mathrm{bi}}$ (Theorem 4.51), we obtain the claim. ☐

Summarizing the results in this subsection, we have the following commutative diagram of isomorphic vector spaces



The composition $\#_Y \circ \rho_{\mathcal{B}}$ should be a Lie algebra isomorphism for the q-Ihara bracket (Definition 3.16) and the uri bracket (Definition 5.10). It is not clear how to find a closed formula for a Lie bracket on the other spaces (resp. in terms of the other alphabets).

5.5 Bimoulds and $\mathfrak{lq}$

We want to relate the space $\mathfrak{lq}$ (Definition 4.57) to bimoulds via the map $\rho_{\mathcal{B}}$ (Definition 5.49) and investigate the obtained properties. This will give the proof that the pair $(\mathfrak{lq}, \{-,-\}_q^D)$ is a Lie algebra (Theorem 4.63).

Theorem 5.68. *For an element $f \in \mathfrak{lq}$, the bimould $\rho_{\mathcal{B}}(f)$ is q-alternal and τ-invariant. More precisely, there is an isomorphism of vector spaces*

$$\mathfrak{lq} \xrightarrow{\sim} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{q\text{-al}},\tau}, \;\; f \mapsto \rho_{\mathcal{B}}(f).$$

The space $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{q\text{-al}},\tau}$ is given in Definition 5.44.

Proof. There is an isomorphism $\mathbb{Q}\langle\mathcal{B}\rangle^0 \backslash \mathbb{Q}\mathbf{1} \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}, \;\; f \mapsto \rho_{\mathcal{B}}(f)$ and by definition a bimould $\rho_{\mathcal{B}}(f) \in \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}$ is q-alternal with coefficient map $\mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q}, \;\; w \mapsto (f \mid w)$ if and only if

$$(f \mid u \sqcup\!\sqcup v) = 0 \text{ for all } u, v \in \mathbb{Q}\langle\mathcal{B}\rangle^0 \backslash \mathbb{Q}\mathbf{1}.$$

By duality (Example A.62) an element in $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ is primitive for $\Delta_{\sqcup\!\sqcup}$ if and only if

$$(f \mid u \sqcup\!\sqcup v) = 0 \text{ for all } u, v \in \mathbb{Q}\langle\mathcal{B}\rangle \backslash \mathbb{Q}\mathbf{1}.$$

Thus for any primitive element $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ (with respect to the coproduct $\Delta_{\sqcup\!\sqcup}$) the bimould $\rho_{\mathcal{B}}(f)$ is q-alternal. On the other hand, the primitive elements of $(\mathbb{Q}\langle\mathcal{B}\rangle, \Delta_{\sqcup\!\sqcup})$ are exactly the elements in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{B}\rangle$ (Corollary A.40). So similar to the map sec_q (Proposition 4.47) we can uniquely recover each element $f \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{B}\rangle$ satisfying $(f \mid b_0) = 0$ from its projection $\Pi_0(f)$. Thus we get an isomorphism

$$\Big\{ f \in \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{B}\rangle \;\Big|\; (f \mid b_0) = 0 \Big\} \to \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{q\text{-al}}, f \mapsto \rho_{\mathcal{B}}(f).$$

As in the proof of Theorem 5.50, $f \in \mathbb{Q}\langle\mathcal{B}\rangle$ satisfies $\tau(\Pi_0(f)) = \Pi_0(f)$ and $(f \mid b_k b_0^m) = 0$ for all $k+m$ even if and only if $\rho_{\mathcal{B}}(f)$ is τ-invariant and $\rho_{\mathcal{B}}(f)_1$ is even. ☐

Corollary 5.69. *There is a vector space isomorphism*

$$\mathfrak{lq} \xrightarrow{\sim} \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}, \quad f \mapsto \rho_{\mathcal{B}}(f)^{\#_Y}.$$

Proof. This is an immediate consequence of Theorem 5.68 and Theorem 5.46. ☐

Since the associated depth-graded space $\mathfrak{lb}$ to $\mathfrak{bm}_0$ (Definition 4.58) is a proper subspace of $\mathfrak{lq}$, we get embedding of vector spaces

$$\mathfrak{lb} \hookrightarrow \mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}, \quad f \mapsto \rho_{\mathcal{B}}(f)^{\#_Y}.$$

Recall that $\mathrm{BARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}},\mathrm{swap}}$ equipped with the ari bracket is a Lie algebra (Theorem 5.26). Thus the ari bracket induces a Lie algebra structure on $\mathfrak{lq}$ under the isomorphism $\#_Y \circ \rho_{\mathcal{B}}$.

Proposition 5.70. *For all $f, g \in \mathbb{Q}\langle\mathcal{B}\rangle$, the following holds*

$$\rho_{\mathcal{B}}\Big(\{f,g\}_q^D\Big)^{\#_Y} = \mathrm{ari}\left(\rho_{\mathcal{B}}(f)^{\#_Y}, \rho_{\mathcal{B}}(g)^{\#_Y}\right).$$

The depth-graded q-Ihara bracket $\{-,-\}_q^D$ is introduced in Definition 4.62.

Proof. Considering the calculations in Theorem 5.52 modulo higher depth leads to

$$\rho_{\mathcal{B}}\left(d_f^{q,D}(g)\right)^{\#_Y} = \operatorname{arit}_{\rho_{\mathcal{B}}(f)^{\#_Y}}\left(\rho_{\mathcal{B}}(g)^{\#_Y}\right), \qquad \rho_{\mathcal{B}}(fg)^{\#_Y} = \operatorname{mu}\left(\rho_{\mathcal{B}}(f)^{\#_Y}, \rho_{\mathcal{B}}(g)^{\#_Y}\right)$$

for all $f, g \in \mathbb{Q}\langle\mathcal{B}\rangle$. Thus, we obtain

$$\begin{aligned}
\rho_{\mathcal{B}}\left(\{f,g\}_q^D\right)^{\#_Y} &= \rho_{\mathcal{B}}\left(d_f^{q,D}(g) - d_g^{q,D}(f) - fg + gf\right)^{\#_Y} \\
&= \operatorname{arit}_{\rho_{\mathcal{B}}(f)^{\#_Y}}\left(\rho_{\mathcal{B}}(g)^{\#_Y}\right) - \operatorname{arit}_{\rho_{\mathcal{B}}(g)^{\#_Y}}\left(\rho_{\mathcal{B}}(f)^{\#_Y}\right) \\
&\quad - \operatorname{mu}\left(\rho_{\mathcal{B}}(f)^{\#_Y}, \rho_{\mathcal{B}}(g)^{\#_Y}\right) + \operatorname{mu}\left(\rho_{\mathcal{B}}(g)^{\#_Y}, \rho_{\mathcal{B}}(f)^{\#_Y}\right) \\
&= \operatorname{ari}\left(\rho_{\mathcal{B}}(f)^{\#_Y}, \rho_{\mathcal{B}}(g)^{\#_Y}\right).
\end{aligned}$$

□

An immediate consequence of Corollary 5.69 and Proposition 5.70 is the following.

Corollary 5.71. *The pair* $(\mathfrak{lq}, \{-,-\}_q^D)$ *is a Lie algebra and there is a Lie algebra isomorphism*

$$\left(\mathfrak{lq}, \{-,-\}_q^D\right) \to \left(\mathrm{BARI}_{\underline{\mathrm{al}},\mathrm{swap}}^{\mathrm{pol},\mathbb{Q}}, \operatorname{ari}\right), \quad f \mapsto \rho_{\mathcal{B}}(f)^{\#_Y}.$$

6 A result towards Bachmann's conjecture in terms of the algebra $\mathbb{Q}\langle\mathcal{B}\rangle^0$

By construction of the balanced multiple q-zeta values (Subsection 2.6), one obtains

$$\begin{aligned}\mathcal{Z}_q &= \operatorname{span}_{\mathbb{Q}}\{\zeta_q(s_1,\dots,s_l) \mid s_1 \geq 1,\ s_2,\dots,s_l \geq 0\},\\ \mathcal{Z}_q^{\circ} &= \operatorname{span}_{\mathbb{Q}}\{\zeta_q(s_1,\dots,s_l) \mid s_1,\dots,s_l \geq 1\}.\end{aligned}$$

Moreover, define the subspaces of bi-brackets (Definition 2.27)

$$\begin{aligned}\mathcal{Z}_q^{+} &= \operatorname{span}_{\mathbb{Q}}\left\{ g\binom{k_1,\dots,k_d}{m_1,\dots,m_d} \;\middle|\; k_1 > m_1,\dots,k_d > m_d \right\},\\ \mathcal{Z}_q^{123} &= \operatorname{span}_{\mathbb{Q}}\left\{ g(k_1,\dots,k_d) \mid k_j \in \{1,2,3\} \right\}.\end{aligned}$$

By definition, there are inclusions

$$\mathcal{Z}_q^{123} \subset \mathcal{Z}_q^{\circ} \subset \mathcal{Z}_q^{+} \subset \mathcal{Z}_q.$$

In [BK20] it is conjectured that all these inclusion are equalities. In this subsection, we will focus on the inclusion $\mathcal{Z}_q^{\circ} \subset \mathcal{Z}_q$, which was already conjectured by H. Bachmann to be an equality ([Ba19, Conjecture 4.3]).

Let $\mathbb{Q}\langle\mathcal{B}\rangle^{\geq 1} \subset \mathbb{Q}\langle\mathcal{B}\rangle^0$ be the free algebra generated by all words in the letters b_i, $i \geq 1$. By Theorem 2.59, we have a surjective algebra morphism

$$\begin{aligned}(\mathbb{Q}\langle\mathcal{B}\rangle^{\geq 1}, *_q) &\twoheadrightarrow (\mathcal{Z}_q^{\circ}, \cdot),\\ b_{k_1}\dots b_{k_d} &\mapsto \zeta_q(k_1,\dots,k_d).\end{aligned}$$

Therefore, a reformulation of Bachmann's conjecture $\mathcal{Z}_q = \mathcal{Z}_q^{\circ}$ is given by the following.

Conjecture 6.1. *There is a surjective algebra morphism*

$$\begin{aligned}(\mathbb{Q}\langle\mathcal{B}\rangle^{\geq 1}, *_q) &\to (\mathcal{Z}_q, \cdot)\\ b_{k_1}\dots b_{k_d} &\mapsto \zeta_q(k_1,\dots,k_d).\end{aligned}$$

Since we expect that all algebraic relations in $\mathcal{Z}_q$ are a consequence of the balanced quasi-shuffle product formula and the τ-invariance of the balanced multiple q-zeta values (Conjecture 2.60), those two properties should be sufficient to prove the surjectivity in Conjecture 6.1.

Remark 6.2. 1) According to the observations on p. 73 et seq., the algebra $(\mathbb{Q}\langle\mathcal{B}\rangle^{\geq 1}, *_q)$ is isomorphic to the usual stuffle algebra $(\mathbb{Q}\langle\mathcal{Y}\rangle, *)$ via the identification $b_i \mapsto y_i$ for $i \geq 1$. Therefore, Conjecture 6.1 would imply the following commutative diagram of algebras

$$\begin{array}{ccccccccc} 0 & \longrightarrow & (\mathbb{Q}\langle\mathcal{Y}\rangle, *) & \hookrightarrow & (\mathbb{Q}\langle\mathcal{B}\rangle, *_q) & \twoheadrightarrow & (\mathbb{Q}\langle\mathcal{X}\rangle, ш) & \longrightarrow & 0\\ & & \big\downarrow{\scriptstyle \zeta_q} & & \big\downarrow{\scriptstyle \zeta_q} & & & & \\ 0 & \longrightarrow & (\mathcal{Z}_q^{\circ}, \cdot) & \xrightarrow{\sim} & (\mathcal{Z}_q, \cdot) & \twoheadrightarrow & 0 & \longrightarrow & 0 \end{array}$$

2) There are some partial results towards Conjecture 6.1 proven in terms of the bi-brackets (Definition 2.27). In [Ba19, Proposition 4.4] Conjecture 6.1 is proven in depth 1 and there is also obtained a partial result towards the depth 2 case. Moreover, in [Vl20] Conjecture 6.1 is shown for depth 2 and odd weight by taking advantage of the fact that any bi-bracket of depth 2 and odd weight is a linear combination of (products of) bi-brackets of depth 1. Finally, there is an approach to Conjecture 6.1 by B. Brindle, which uses the SZ multiple q-zeta values (Definition 2.9).

Definition 6.3. For any word $w = b_{k_1} b_0^{m_1} \dots b_{k_d} b_0^{m_d} \in \mathbb{Q}\langle \mathcal{B} \rangle^0$, let

$$\mathrm{b}(w) = \min\{k_1 + \dots + k_d - d, m_1 + \dots + m_d\}.$$

By definition, a word $w \in \mathbb{Q}\langle \mathcal{B} \rangle^0$ satisfies $\mathrm{b}(w) = 0$ if and only if w is contained in $\mathbb{Q}\langle \mathcal{B} \rangle^{\geq 1}$ or only consists of the letters b_0, b_1. One obtains

$$\tau(b_1 b_0^{m_1} \dots b_1 b_0^{m_d}) = b_{m_d+1} \dots b_{m_1+1}$$

for all $m_1, \dots, m_d \geq 0$. Therefore, applying the τ-invariance of the balanced multiple q-zeta values shows that $\zeta_q(w) \in \mathcal{Z}_q^\circ$ for any word $w \in \mathbb{Q}\langle \mathcal{B} \rangle^0$ satisfying $\mathrm{b}(w) = 0$.

Theorem 6.4. *Let $w \in \mathbb{Q}\langle \mathcal{B} \rangle^0$ be a word satisfying $\mathrm{b}(w) = 1$, then $\zeta_q(w) \in \mathcal{Z}_q^\circ$.*

In particular, any balanced multiple q-zeta value of the form

$$\zeta_q(k_1, \dots, k_i, 0, k_{i+1}, \dots, k_d), \qquad k_1, \dots, k_d \geq 1, \ i \in \{1, \dots, d\},$$

is contained in $\mathcal{Z}_q^\circ$.

Proof. We use induction on the depth. Let $w \in \mathbb{Q}\langle \mathcal{B} \rangle^0$ be a word of depth 1 satisfying $\mathrm{b}(w) = 1$, i.e., we have $w = b_{m+1} b_0$ or $w = b_2 b_0^m$ for some $m \geq 1$. Since $\tau(b_{m+1} b_0) = b_2 b_0^m$ and the balanced multiple q-zeta values are τ-invariant, it is enough to show that $\zeta_q(w) \in \mathcal{Z}_q^\circ$ for $w = b_2 b_0^m$. Compute

$$b_1 b_0^m *_q b_1 = \sum_{i=0}^{m} b_1 b_0^i b_1 b_0^{m-i} + b_1^2 b_0^m + b_2 b_0^m.$$

Since $\zeta_q : (\mathbb{Q}\langle \mathcal{B} \rangle^0, *_q) \to \mathcal{Z}_q$ is an algebra morphism (Theorem 2.59), we deduce

$$\zeta_q(w) = \zeta_q(b_1 b_0^m) \zeta_q(b_1) - \sum_{i=0}^{m} \zeta_q(b_1 b_0^i b_1 b_0^{m-i}) - \zeta_q(b_1^2 b_0^m).$$

Any word u contained in the right-hand side satisfies $b(u) = 0$ and hence is contained in $\mathcal{Z}_q^\circ$. Therefore, we have $\zeta_q(w) \in \mathcal{Z}_q^\circ$.
Assume that for all words $w \in \mathbb{Q}\langle \mathcal{B} \rangle^0$ of depth $d \geq 1$ satisfying $\mathrm{b}(w) = 1$, the element $\zeta_q(w)$ is contained in $\mathcal{Z}_q^\circ$. Let $n, m_1, \dots, m_d \geq 0$, then for $i = 1, \dots, d$, one obtains

$$\begin{aligned} &b_{n+1} *_q b_{m_1+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_d} \\ &\qquad \equiv \sum_{j=0}^{i} b_{m_1+1} \dots b_{m_j+1} b_{n+1} b_{m_{j+1}+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_d} \\ &\qquad + \sum_{j=i}^{d} b_{m_1+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_j+1} b_{n+1} b_{m_{j+1}+1} \dots b_{m_d} \\ &\qquad \mod \ \text{depth} \ \leq d. \end{aligned}$$

By the induction hypothesis, we have $\zeta_q(b_{n+1}) \zeta_q(b_{m_1+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_d}) \in \mathcal{Z}_q^\circ$. Moreover, all words w of depth $\leq d$ appearing in these products also satisfy $b(w) = 1$, thus they are also contained in $\mathcal{Z}_q^\circ$ by the induction hypothesis. We deduce

$$\begin{aligned} \sum_{i=1}^{d} \Bigg(&\sum_{j=0}^{i} \zeta_q(b_{m_1+1} \dots b_{m_j+1} b_{n+1} b_{m_{j+1}+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_d}) \\ &+ \sum_{j=i}^{d} \zeta_q(b_{m_1+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_j+1} b_{n+1} b_{m_{j+1}+1} \dots b_{m_d}) \Bigg) \in \mathcal{Z}_q^\circ. \end{aligned} \tag{6.4.1}$$

On the other hand, we obtain for $j = 0, \dots, d$ that

$$
\begin{aligned}
b_1 *_q b_1 b_0^{m_d} \dots b_1 b_0^{m_{j+1}} b_1 b_0^n b_1 b_0^{m_j} \dots b_1 b_0^{m_1} \equiv \\
&\sum_{i=1}^{j} b_1 b_0^{m_d} \dots b_1 b_0^{m_{j+1}} b_1 b_0^n b_1 b_0^{m_j} \dots b_1 b_0^{m_{i+1}} b_2 b_0^{m_i} b_1 b_0^{m_{i-1}} \dots b_1 b_0^{m_1} \\
&+ b_1 b_0^{m_d} \dots b_1 b_0^{m_{j+1}} b_2 b_0^n b_1 b_0^{m_j} \dots b_1 b_0^{m_1} \\
&+ \sum_{i=j}^{d} b_1 b_0^{m_d} \dots b_1 b_0^{m_{i+1}} b_2 b_0^{m_i} b_1 b_0^{m_{i-1}} \dots b_1 b_0^{m_{j+1}} b_1 b_0^n b_1 b_0^{m_j} \dots b_1 b_0^{m_1} \\
&\quad \text{mod} \;\; \text{words } w \text{ satisfying } b(w) = 0.
\end{aligned}
$$

Since all words $w \in \mathbb{Q}\langle\mathcal{B}\rangle^0$ satisfying $b(w) = 0$ are contained in $\mathcal{Z}_q^\circ$, we obtain

$$
\zeta_q(b_1)\zeta_q(b_1 b_0^{m_d} \dots b_1 b_0^{m_{j+1}} b_1 b_0^n b_1 b_0^{m_j} \dots b_1 b_0^{m_1}) \in \mathcal{Z}_q^\circ
$$

and thus by applying the τ-invariance of the balanced multiple q-zeta values

$$
\begin{aligned}
\sum_{j=0}^{d} \Bigg(&\sum_{i=1}^{j} \zeta_q(b_{m_1+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_j+1} b_{n+1} b_{m_{j+1}+1} \dots b_{m_d+1}) \\
&+ \zeta_q(b_{m_1+1} \dots b_{m_j+1} b_{n+1} b_0 b_{m_{j+1}+1} \dots b_{m_d+1}) \\
&+ \sum_{i=j}^{d} \zeta_q(b_{m_1+1} \dots b_{m_j+1} b_{n+1} b_{m_{j+1}+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_d+1}) \Bigg) \in \mathcal{Z}_q^\circ.
\end{aligned} \tag{6.4.2}
$$

The two expressions given in (6.4.1) and (6.4.2) are equal up to the additional term $\zeta_q(b_{n+1} b_0 b_{m_1+1} \dots b_{m_d+1})$ appearing in (6.4.2), therefore we get by subtracting them

$$
\zeta_q(b_{n+1} b_0 b_{m_1+1} \dots b_{m_d+1}) \in \mathcal{Z}_q^\circ. \tag{6.4.3}
$$

Next, let $n_1, n_2, m_1, \dots, m_{d-1} \geq 0$. Then compute all products

$$
b_{n_1+1} b_{n_2+1} *_q b_{m_1+1} \dots b_{m_i+1} b_0 b_{m_{i+1}+1} \dots b_{m_{d-1}+1}, \qquad i = 1, \dots, d-1. \tag{6.4.4}
$$

As before, by the induction hypothesis each product gives a linear combination of balanced multiple q-zeta values contained in $\mathcal{Z}_q^\circ$. Similarly, for $0 \leq j_1 \leq j_2 \leq d-1$ compute the products

$$
b_1 *_q b_1 b_0^{m_{d-1}} \dots b_1 b_0^{m_{j_2+1}} b_1 b_{n_2} b_1 b_0^{m_{j_1}} \dots b_1 b_0^{m_{j_1+1}} b_1 b_0^{n_1} b_1 b_0^{m_{j_2}} \dots b_1 b_0^{m_1}. \tag{6.4.5}
$$

Since the words w appearing in the products satisfy $b(w) = 0$, we obtain as in the previous case linear combinations of balanced multiple q-zeta values contained in $\mathcal{Z}_q^\circ$. Again we obtain that the sum of all expressions obtained from (6.4.4) equals the sum of all expressions obtained from (6.4.5) except for some additional terms (appearing in (6.4.5)), explicitly we get

$$
\begin{aligned}
&\zeta_q(b_{n_1+1} b_{n_2+1} b_0 b_{m_1+1} \dots b_{m_{d-1}+1}) \\
&\qquad + \sum_{j=0}^{d-1} \zeta_q(b_{n_1+1} b_0 b_{m_1+1} \dots b_{m_j+1} b_{n_2+1} b_{m_{j+1}+1} \dots b_{m_{d-1}+1}) \in \mathcal{Z}_q^\circ.
\end{aligned}
$$

From the first case (6.4.3) we get $\zeta_q(b_{n_1+1} b_0 b_{m_1+1} \dots b_{m_j+1} b_{n_2+1} b_{m_{j+1}+1} \dots b_{m_{d-1}+1}) \in \mathcal{Z}_q^\circ$ for each $j = 0, \dots, d-1$ and thus, we deduce

$$
\zeta_q(b_{n_1+1} b_{n_2+1} b_0 b_{m_1+1} \dots b_{m_{d-1}+1}) \in \mathcal{Z}_q^\circ.
$$

Iterating this process shows that any balanced multiple q-zeta value of the form

$$\zeta_q(b_{m_1+1}\dots b_{m_i+1}b_0b_{m_{i+1}+1}\dots b_{m_{d+1}+1}), \qquad i=1,\dots,d+1,$$

is contained in $\mathcal{Z}_q^\circ$. Applying the τ-invariance of the balanced multiple q-zeta values shows that also

$$\zeta_q(b_1b_0^{m_1}\dots b_1b_0^{m_j}b_2b_0^{m_{j+1}}b_1b_0^{m_{j+2}}\dots b_1b_0^{m_{d+1}}), \qquad j=0,\dots,d+1,$$

is contained in $\mathcal{Z}_q^\circ$. Since any word $w\in\mathbb{Q}\langle\mathcal{B}\rangle^0$ of depth $d+1$ satisfying $b(w)=1$ has one of the above given two shapes, we have $\zeta_q(w)\in\mathcal{Z}_q^\circ$ for all words $w\in\mathbb{Q}\langle\mathcal{B}\rangle^0$ of depth $d+1$ satisfying $b(w)=1$. □

Example 6.5. We will illustrate the idea of proof explicitly in depth 4. In particular, we assume that any word $w\in\mathbb{Q}\langle\mathcal{B}\rangle^0$ of depth <4 with $b(w)=1$ satisfies $\zeta_q(w)\in\mathcal{Z}_q^\circ$.

Let $n,m_1,m_2,m_3\geq 0$. We compute

$$\begin{aligned}
b_{n+1}*_q b_{m_1+1}b_0b_{m_2+1}b_{m_3+1} \equiv\ & b_{n+1}b_{m_1+1}b_0b_{m_2+1}b_{m_3+1}+b_{m_1+1}b_{n+1}b_0b_{m_2+1}b_{m_3+1}\\
&+b_{m_1+1}b_0b_{n+1}b_{m_2+1}b_{m_3+1}+b_{m_1+1}b_0b_{m_2+1}b_{n+1}b_{m_3+1}\\
&+b_{m_1+1}b_0b_{m_2+1}b_{m_3+1}b_{n+1} \mod \text{depth } <4,\\
b_{n+1}*_q b_{m_1+1}b_{m_2+1}b_0b_{m_3+1} \equiv\ & b_{n+1}b_{m_1+1}b_{m_2+1}b_0b_{m_3+1}+b_{m_1+1}b_{n+1}b_{m_2+1}b_0b_{m_3+1}\\
&+b_{m_1+1}b_{m_2+1}b_{n+1}b_0b_{m_3+1}+b_{m_1+1}b_{m_2+1}b_0b_{n+1}b_{m_3+1}\\
&+b_{m_1+1}b_{m_2+1}b_0b_{m_3+1}b_{n+1} \mod \text{depth } <4,\\
b_{n+1}*_q b_{m_1+1}b_{m_2+1}b_{m_3+1}b_0 \equiv\ & b_{n+1}b_{m_1+1}b_{m_2+1}b_{m_3+1}b_0+b_{m_1+1}b_{n+1}b_{m_2+1}b_{m_3+1}b_0\\
&+b_{m_1+1}b_{m_2+1}b_{n+1}b_{m_3+1}b_0+b_{m_1+1}b_{m_2+1}b_{m_3+1}b_{n+1}b_0\\
&+b_{m_1+1}b_{m_2+1}b_{m_3+1}b_{n+1}b_0 \mod \text{depth } <4.
\end{aligned}$$

All appearing words w of depth <4 satisfy $b(w)=1$, so by assumption, those are contained in $\mathcal{Z}_q^\circ$. Moreover, also the products are contained in $\mathcal{Z}_q^\circ$ by assumption, thus by summing up the three equations, we get

$$\begin{aligned}
&\zeta_q(b_{n+1}b_{m_1+1}b_0b_{m_2+1}b_{m_3+1})+\zeta_q(b_{m_1+1}b_{n+1}b_0b_{m_2+1}b_{m_3+1})+\zeta_q(b_{m_1+1}b_0b_{n+1}b_{m_2+1}b_{m_3+1})\\
&+\zeta_q(b_{m_1+1}b_0b_{m_2+1}b_{n+1}b_{m_3+1})+\zeta_q(b_{m_1+1}b_0b_{m_2+1}b_{m_3+1}b_{n+1})+\zeta_q(b_{n+1}b_{m_1+1}b_{m_2+1}b_0b_{m_3+1})\\
&+\zeta_q(b_{m_1+1}b_{n+1}b_{m_2+1}b_0b_{m_3+1})+\zeta_q(b_{m_1+1}b_{m_2+1}b_{n+1}b_0b_{m_3+1})+\zeta_q(b_{m_1+1}b_{m_2+1}b_0b_{n+1}b_{m_3+1})\\
&+\zeta_q(b_{m_1+1}b_{m_2+1}b_0b_{m_3+1}b_{n+1})+\zeta_q(b_{n+1}b_{m_1+1}b_{m_2+1}b_{m_3+1}b_0)+\zeta_q(b_{m_1+1}b_{n+1}b_{m_2+1}b_{m_3+1}b_0)\\
&+\zeta_q(b_{m_1+1}b_{m_2+1}b_{n+1}b_{m_3+1}b_0)+\zeta_q(b_{m_1+1}b_{m_2+1}b_{m_3+1}b_{n+1}b_0)+\zeta_q(b_{m_1+1}b_{m_2+1}b_{m_3+1}b_{n+1}b_0)\\
&\quad\in\mathcal{Z}_q^\circ. \qquad (6.5.1)
\end{aligned}$$

On the other hand, we have

$$\begin{aligned} b_1 *_q b_1 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{m_1} b_1 b_0^{n} \equiv\ & b_2 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{m_1} b_1 b_0^{n} + b_1 b_0^{m_3} b_2 b_0^{m_2} b_1 b_0^{m_1} b_1 b_0^{n} \\ & + b_1 b_0^{m_3} b_1 b_0^{m_2} b_2 b_0^{m_1} b_1 b_0^{n} + b_1 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{m_1} b_2 b_0^{n} \\ & \mod \text{ words } w \text{ satisfying } b(w) = 0, \\ b_1 *_q b_1 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{n} b_1 b_0^{m_1} \equiv\ & b_2 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{n} b_1 b_0^{m_1} + b_1 b_0^{m_3} b_2 b_0^{m_2} b_1 b_0^{n} b_1 b_0^{m_1} \\ & + b_1 b_0^{m_3} b_1 b_0^{m_2} b_2 b_0^{n} b_1 b_0^{m_1} + b_1 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{n} b_2 b_0^{m_1} \\ & \mod \text{ words } w \text{ satisfying } b(w) = 0, \\ b_1 *_q b_1 b_0^{m_3} b_1 b_0^{n} b_1 b_0^{m_2} b_1 b_0^{m_1} \equiv\ & b_2 b_0^{m_3} b_1 b_0^{n} b_1 b_0^{m_2} b_1 b_0^{m_1} + b_1 b_0^{m_3} b_2 b_0^{n} b_1 b_0^{m_2} b_1 b_0^{m_1} \\ & + b_1 b_0^{m_3} b_1 b_0^{n} b_2 b_0^{m_2} b_1 b_0^{m_1} + b_1 b_0^{m_3} b_1 b_0^{n} b_1 b_0^{m_2} b_2 b_0^{m_1} \\ & \mod \text{ words } w \text{ satisfying } b(w) = 0, \\ b_1 *_q b_1 b_0^{n} b_1 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{m_1} \equiv\ & b_2 b_0^{n} b_1 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{m_1} + b_1 b_0^{n} b_2 b_0^{m_3} b_1 b_0^{m_2} b_1 b_0^{m_1} \\ & + b_1 b_0^{n} b_1 b_0^{m_3} b_2 b_0^{m_2} b_1 b_0^{m_1} + b_1 b_0^{n} b_1 b_0^{m_3} b_1 b_0^{m_2} b_2 b_0^{m_1} \\ & \mod \text{ words } w \text{ satisfying } b(w) = 0. \end{aligned}$$

For all words $w \in \mathbb{Q}\langle \mathcal{B} \rangle^0$ satisfying $b(w) = 0$, we have $\zeta_q(w) \in \mathcal{Z}_q^\circ$. In particular, all products are contained in $\mathcal{Z}_q^\circ$. Therefore, by summing up the four product expressions and applying the τ-invariance of the balanced multiple q-zeta values, we obtain

$$\begin{aligned} & \zeta_q(b_{n+1} b_{m_1+1} b_{m_2+1} b_{m_3+1} b_0) + \zeta_q(b_{n+1} b_{m_1+1} b_{m_2+1} b_0 b_{m_3+1}) + \zeta_q(b_{n+1} b_{m_1+1} b_0 b_{m_2+1} b_{m_3+1}) \\ & + \zeta_q(b_{n+1} b_0 b_{m_1+1} b_{m_2+1} b_{m_3+1}) + \zeta_q(b_{m_1+1} b_{n+1} b_{m_2+1} b_{m_3+1} b_0) + \zeta_q(b_{m_1+1} b_{n+1} b_{m_2+1} b_0 b_{m_3+1}) \\ & + \zeta_q(b_{m_1+1} b_{n+1} b_0 b_{m_2+1} b_{m_3+1}) + \zeta_q(b_{m_1+1} b_0 b_{n+1} b_{m_2+1} b_{m_3+1}) + \zeta_q(b_{m_1+1} b_{m_2+1} b_{n+1} b_{m_3+1} b_0) \\ & + \zeta_q(b_{m_1+1} b_{m_2+1} b_{n+1} b_0 b_{m_3+1}) + \zeta_q(b_{m_1+1} b_{m_2+1} b_0 b_{n+1} b_{m_3+1}) + \zeta_q(b_{m_1+1} b_0 b_{m_2+1} b_{n+1} b_{m_3+1}) \\ & + \zeta_q(b_{m_1+1} b_{m_2+1} b_{m_3+1} b_{n+1} b_0) + \zeta_q(b_{m_1+1} b_{m_2+1} b_{m_3+1} b_0 b_{n+1}) + \zeta_q(b_{m_1+1} b_{m_2+1} b_0 b_{m_3+1} b_{n+1}) \\ & + \zeta_q(b_{m_1+1} b_0 b_{m_2+1} b_{m_3+1} b_{n+1}) \quad \in \mathcal{Z}_q^\circ. \end{aligned} \tag{6.5.2}$$

The expressions in (6.5.1) and 6.5.2 only differ by the term $\zeta_q(b_{n+1} b_0 b_{m_1+1} b_{m_2+1} b_{m_3+1})$, in particular subtracting (6.5.1) from (6.5.2) yields

$$\zeta_q(b_{n+1} b_0 b_{m_1+1} b_{m_2+1} b_{m_3+1}) \in \mathcal{Z}_q^\circ. \tag{6.5.3}$$

Next, let $n_1, n_2, m_1, m_2 \geq 0$. Again we compute

$$\begin{aligned} b_{n_1+1} b_{n_2+1} *_q b_{m_1+1} b_0 b_{m_2+1} \equiv\ & b_{n_1+1} b_{n_2+1} b_{m_1+1} b_0 b_{m_2+1} + b_{n_1+1} b_{m_1+1} b_{n_2+1} b_0 b_{m_2+1} \\ & + b_{n_1+1} b_{m_1+1} b_0 b_{n_2+1} b_{m_2+1} + b_{n_1+1} b_{m_1+1} b_0 b_{m_2+1} b_{n_2+1} \\ & + b_{m_1+1} b_{n_1+1} b_{n_2+1} b_0 b_{m_2+1} + b_{m_1+1} b_{n_1+1} b_0 b_{n_2+1} b_{m_2+1} \\ & + b_{m_1+1} b_{n_1+1} b_0 b_{m_2+1} b_{n_2+1} + b_{m_1+1} b_0 b_{n_1+1} b_{n_2+1} b_{m_2+1} \\ & + b_{m_1+1} b_0 b_{n_1+1} b_{m_2+1} b_{n_2+1} + b_{m_1+1} b_0 b_{m_2+1} b_{n_1+1} b_{n_2+1} \\ & \mod \text{ depth } < 4, \\ b_{n_1+1} b_{n_2+1} *_q b_{m_1+1} b_{m_2+1} b_0 \equiv\ & b_{n_1+1} b_{n_2+1} b_{m_1+1} b_{m_2+1} b_0 + b_{n_1+1} b_{m_1+1} b_{n_2+1} b_{m_2+1} b_0 \\ & + b_{n_1+1} b_{m_1+1} b_{m_2+1} b_{n_2+1} b_0 + b_{n_1+1} b_{m_1+1} b_{m_2+1} b_0 b_{n_2+1} \\ & + b_{m_1+1} b_{n_1+1} b_{n_2+1} b_{m_2+1} b_0 + b_{m_1+1} b_{n_1+1} b_{m_2+1} b_{n_2+1} b_0 \\ & + b_{m_1+1} b_{n_1+1} b_{m_2+1} b_0 b_{n_2+1} + b_{m_1+1} b_{m_2+1} b_{n_1+1} b_{n_2+1} b_0 \\ & + b_{m_1+1} b_{m_2+1} b_{n_1+1} b_0 b_{n_2+1} + b_{m_1+1} b_{m_2+1} b_0 b_{n_1+1} b_{n_2+1} \\ & \mod \text{ depth } < 4. \end{aligned}$$

Then by the completely same argument as before, we deduce that

$$\begin{aligned}
&\zeta_q(b_{n_1+1}b_{n_2+1}b_{m_1+1}b_0b_{m_2+1}) + \zeta_q(b_{n_1+1}b_{m_1+1}b_{n_2+1}b_0b_{m_2+1}) + \zeta_q(b_{n_1+1}b_{m_1+1}b_0b_{n_2+1}b_{m_2+1}) \\
&+ \zeta_q(b_{n_1+1}b_{m_1+1}b_0b_{m_2+1}b_{n_2+1}) + \zeta_q(b_{m_1+1}b_{n_1+1}b_{n_2+1}b_0b_{m_2+1}) + \zeta_q(b_{m_1+1}b_{n_1+1}b_0b_{n_2+1}b_{m_2+1}) \\
&+ \zeta_q(b_{m_1+1}b_{n_1+1}b_0b_{m_2+1}b_{n_2+1}) + \zeta_q(b_{m_1+1}b_0b_{n_1+1}b_{n_2+1}b_{m_2+1}) + \zeta_q(b_{m_1+1}b_0b_{n_1+1}b_{m_2+1}b_{n_2+1}) \\
&+ \zeta_q(b_{m_1+1}b_0b_{m_2+1}b_{n_1+1}b_{n_2+1}) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{m_1+1}b_{m_2+1}b_0) + \zeta_q(b_{n_1+1}b_{m_1+1}b_{n_2+1}b_{m_2+1}b_0) \\
&+ \zeta_q(b_{n_1+1}b_{m_1+1}b_{m_2+1}b_{n_2+1}b_0) + \zeta_q(b_{n_1+1}b_{m_1+1}b_{m_2+1}b_0b_{n_2+1}) + \zeta_q(b_{m_1+1}b_{n_1+1}b_{n_2+1}b_{m_2+1}b_0) \\
&+ \zeta_q(b_{m_1+1}b_{n_1+1}b_{m_2+1}b_{n_2+1}b_0) + \zeta_q)b_{m_1+1}b_{n_1+1}b_{m_2+1}b_0b_{n_2+1}) + \zeta_q(b_{m_1+1}b_{m_2+1}b_{n_1+1}b_{n_2+1}b_0) \\
&+ \zeta_q(b_{m_1+1}b_{m_2+1}b_{n_1+1}b_0b_{n_2+1}) + \zeta_q(b_{m_1+1}b_{m_2+1}b_0b_{n_1+1}b_{n_2+1}) \quad \in \mathcal{Z}_q^\circ. \qquad (6.5.4)
\end{aligned}$$

On the other hand, we compute

$$\begin{aligned}
b_1 *_q b_1b_0^{m_2}b_1b_0^{m_1}b_1b_0^{n_2}b_1b_0^{n_1} \equiv\ & b_2b_0^{m_2}b_1b_0^{m_1}b_1b_0^{n_2}b_1b_0^{n_1} + b_1b_0^{m_2}b_2b_0^{m_1}b_1b_0^{n_2}b_1b_0^{n_1} \\
& + b_1b_0^{m_2}b_1b_0^{m_1}b_2b_0^{n_2}b_1b_0^{n_1} + b_1b_0^{m_2}b_1b_0^{m_1}b_1b_0^{n_2}b_2b_0^{n_1} \\
& \mod \text{ words } w \text{ satisfying } b(w)=0, \\
b_1 *_q b_1b_0^{m_2}b_1b_0^{n_2}b_1b_0^{m_1}b_1b_0^{n_1} \equiv\ & b_2b_0^{m_2}b_1b_0^{n_2}b_1b_0^{m_1}b_1b_0^{n_1} + b_1b_0^{m_2}b_2b_0^{n_2}b_1b_0^{m_1}b_1b_0^{n_1} \\
& + b_1b_0^{m_2}b_1b_0^{n_2}b_2b_0^{m_1}b_1b_0^{n_1} + b_1b_0^{m_2}b_1b_0^{n_2}b_1b_0^{m_1}b_2b_0^{n_1} \\
& \mod \text{ words } w \text{ satisfying } b(w)=0, \\
b_1 *_q b_1b_0^{n_2}b_1b_0^{m_2}b_1b_0^{m_1}b_1b_0^{n_1} \equiv\ & b_2b_0^{n_2}b_1b_0^{m_2}b_1b_0^{m_1}b_1b_0^{n_1} + b_1b_0^{n_2}b_2b_0^{m_2}b_1b_0^{m_1}b_1b_0^{n_1} \\
& + b_1b_0^{n_2}b_1b_0^{m_2}b_2b_0^{m_1}b_1b_0^{n_1} + b_1b_0^{n_2}b_1b_0^{m_2}b_1b_0^{m_1}b_2b_0^{n_1} \\
& \mod \text{ words } w \text{ satisfying } b(w)=0, \\
b_1 *_q b_1b_0^{m_2}b_1b_0^{n_2}b_1b_0^{n_1}b_1b_0^{m_1} \equiv\ & b_2b_0^{m_2}b_1b_0^{n_2}b_1b_0^{n_1}b_1b_0^{m_1} + b_1b_0^{m_2}b_2b_0^{n_2}b_1b_0^{n_1}b_1b_0^{m_1} \\
& + b_1b_0^{m_2}b_1b_0^{n_2}b_2b_0^{n_1}b_1b_0^{m_1} + b_1b_0^{m_2}b_1b_0^{n_2}b_1b_0^{n_1}b_2b_0^{m_1} \\
& \mod \text{ words } w \text{ satisfying } b(w)=0, \\
b_1 *_q b_1b_0^{n_2}b_1b_0^{m_2}b_1b_0^{n_1}b_1b_0^{m_1} \equiv\ & b_2b_0^{n_2}b_1b_0^{m_2}b_1b_0^{n_1}b_1b_0^{m_1} + b_1b_0^{n_2}b_2b_0^{m_2}b_1b_0^{n_1}b_1b_0^{m_1} \\
& + b_1b_0^{n_2}b_1b_0^{m_2}b_2b_0^{n_1}b_1b_0^{m_1} + b_1b_0^{n_2}b_1b_0^{m_2}b_1b_0^{n_1}b_2b_0^{m_1} \\
& \mod \text{ words } w \text{ satisfying } b(w)=0, \\
b_1 *_q b_1b_0^{n_2}b_1b_0^{n_1}b_1b_0^{m_2}b_1b_0^{m_1} \equiv\ & b_2b_0^{n_2}b_1b_0^{n_1}b_1b_0^{m_2}b_1b_0^{m_1} + b_1b_0^{n_2}b_2b_0^{n_1}b_1b_0^{m_2}b_1b_0^{m_1} \\
& + b_1b_0^{n_2}b_1b_0^{n_1}b_2b_0^{m_2}b_1b_0^{m_1} + b_1b_0^{n_2}b_1b_0^{n_1}b_1b_0^{m_2}b_2b_0^{m_1} \\
& \mod \text{ words } w \text{ satisfying } b(w)=0.
\end{aligned}$$

Again using the same arguments as before and applying the τ-invariance of the balanced multiple q-zeta values yields

$$\begin{aligned}
&\zeta_q(b_{n_1+1}b_{n_2+1}b_{m_1+1}b_{m_2+1}b_0) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{m_1+1}b_0b_{m_2+1}) + \zeta_q(b_{n_1+1}b_{n_2+1}b_0b_{m_1+1}b_{m_2+1}) \\
&+ \zeta_q(b_{n_1+1}b_0b_{n_2+1}b_{m_1+1}b_{m_2+1}) + \zeta_q(b_{n_1+1}b_{m_1+1}b_{n_2+1}b_{m_2+1}b_0) + \zeta_q(b_{n_1+1}b_{m_1+1}b_{n_2+1}b_0b_{m_2+1}) \\
&+ \zeta_q(b_{n_1+1}b_{m_1+1}b_0b_{n_2+1}b_{m_2+1}) + \zeta_q(b_{n_1+1}b_0b_{m_1+1}b_{n_2+1}b_{m_2+1}) + \zeta_q(b_{n_1+1}b_{m_1+1}b_{m_2+1}b_{n_2+1}b_0) \\
&+ \zeta_q(b_{n_1+1}b_{m_1+1}b_{m_2+1}b_0b_{n_2+1}) + \zeta_q(b_{n_1+1}b_{m_1+1}b_0b_{m_2+1}b_{n_2+1}) + \zeta_q(b_{n_1+1}b_0b_{m_1+1}b_{m_2+1}b_{n_2+1}) \\
&+ \zeta_q(b_{m_1+1}b_{n_1+1}b_{n_2+1}b_{m_2+1}b_0) + \zeta_q(b_{m_1+1}b_{n_1+1}b_{n_2+1}b_0b_{m_2+1}) + \zeta_q(b_{m_1+1}b_{n_1+1}b_0b_{n_2+1}b_{m_2+1}) \\
&+ \zeta_q(b_{m_1+1}b_0b_{n_1+1}b_{n_2+1}b_{m_2+1}) + \zeta_q(b_{m_1+1}b_{n_1+1}b_{m_2+1}b_{n_2+1}b_0) + \zeta_q(b_{m_1+1}b_{n_1+1}b_{m_2+1}b_0b_{n_2+1}) \\
&+ \zeta_q(b_{m_1+1}b_{n_1+1}b_0b_{m_2+1}b_{n_2+1}) + \zeta_q(b_{m_1+1}b_0b_{n_1+1}b_{m_2+1}b_{n_2+1}) + \zeta_q(b_{m_1+1}b_{m_2+1}b_{n_1+1}b_{n_2+1}b_0) \\
&+ \zeta_q(b_{m_1+1}b_{m_2+1}b_{n_1+1}b_0b_{n_2+1}) + \zeta_q(b_{m_1+1}b_{m_2+1}b_0b_{n_1+1}b_{n_2+1}) + \zeta_q(b_{m_1+1}b_0b_{m_2+1}b_{n_1+1}b_{n_2+1}) \\
&\in \mathcal{Z}_q^\circ \qquad (6.5.5)
\end{aligned}$$

Subtracting (6.5.4) from (6.5.5) then yields

$$\zeta_q(b_{n_1+1}b_0b_{n_2+1}b_{m_1+1}b_{m_2+1}) + \zeta_q(b_{n_1+1}b_0b_{m_1+1}b_{n_2+1}b_{m_2+1}) + \zeta_q(b_{n_1+1}b_0b_{m_1+1}b_{m_2+1}b_{n_2+1})$$
$$+ \zeta_q(b_{n_1+1}b_{n_2+1}b_0b_{m_1+1}b_{m_2+1}) \quad \in \mathcal{Z}_q^\circ$$

Applying the result from the first case (6.5.3) then gives

$$\zeta_q(b_{n_1+1}b_{n_2+1}b_0b_{m_1+1}b_{m_2+1}) \in \mathcal{Z}_q^\circ \tag{6.5.6}$$

Next, let $n_1, n_2, n_3, m \geq 0$. As before, we compute

$$\begin{aligned} b_{n_1+1}b_{n_2+1}b_{n_3+1} *_q b_{m+1}b_0 \equiv\ & b_{n_1+1}b_{n_2+1}b_{n_3+1}b_{m+1}b_0 + b_{n_1+1}b_{n_2+1}b_{m+1}b_{n_3+1}b_0 \\ & + b_{n_1+1}b_{m+1}b_{n_2+1}b_{n_3+1}b_0 + b_{m+1}b_{n_1+1}b_{n_2+1}b_{n_3+1}b_0 \\ & + b_{n_1+1}b_{n_2+1}b_{m+1}b_0b_{n_3+1} + b_{n_1+1}b_{m+1}b_{n_2+1}b_0b_{n_3+1} \\ & + b_{m+1}b_{n_1+1}b_{n_2+1}b_0b_{n_3+1} + b_{n_1+1}b_{m+1}b_0b_{n_2+1}b_{n_3+1} \\ & + b_{m+1}b_{n_1+1}b_0b_{n_2+1}b_{n_3+1} + b_{m+1}b_0b_{n_1+1}b_{n_2+1}b_{n_3+1} \\ & \mod \text{ depth } < 4 \end{aligned}$$

and deduce

$$\begin{aligned} & \zeta_q(b_{n_1+1}b_{n_2+1}b_{n_3+1}b_{m+1}b_0) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{m+1}b_{n_3+1}b_0) + \zeta_q(b_{n_1+1}b_{m+1}b_{n_2+1}b_{n_3+1}b_0) \\ & + \zeta_q(b_{m+1}b_{n_1+1}b_{n_2+1}b_{n_3+1}b_0) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{m+1}b_0b_{n_3+1}) + \zeta_q(b_{n_1+1}b_{m+1}b_{n_2+1}b_0b_{n_3+1}) \\ & + \zeta_q(b_{m+1}b_{n_1+1}b_{n_2+1}b_0b_{n_3+1}) + \zeta_q(b_{n_1+1}b_{m+1}b_0b_{n_2+1}b_{n_3+1}) + \zeta_q(b_{m+1}b_{n_1+1}b_0b_{n_2+1}b_{n_3+1}) \\ & + \zeta_q(b_{m+1}b_0b_{n_1+1}b_{n_2+1}b_{n_3+1}) \quad \in \mathcal{Z}_q^\circ \end{aligned} \tag{6.5.7}$$

On the other hand, we have

$$\begin{aligned} b_1 *_q b_1b_0^m b_1b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1} \equiv\ & b_2b_0^m b_1b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1} + b_1b_0^m b_2b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1} \\ & + b_1b_0^m b_1b_0^{n_3}b_2b_0^{n_2}b_1b_0^{n_1} + b_1b_0^m b_1b_0^{n_3}b_1b_0^{n_2}b_2b_0^{n_1} \\ & \mod \text{ words } w \text{ satisfying } b(w) = 0, \\ b_1 *_q b_1b_0^{n_3}b_1b_0^m b_1b_0^{n_2}b_1b_0^{n_1} \equiv\ & b_2b_0^{n_3}b_1b_0^m b_1b_0^{n_2}b_1b_0^{n_1} + b_1b_0^{n_3}b_2b_0^m b_1b_0^{n_2}b_1b_0^{n_1} \\ & + b_1b_0^{n_3}b_1b_0^m b_2b_0^{n_2}b_1b_0^{n_1} + b_1b_0^{n_3}b_1b_0^m b_1b_0^{n_2}b_2b_0^{n_1} \\ & \mod \text{ words } w \text{ satisfying } b(w) = 0, \\ b_1 *_q b_1b_0^{n_3}b_1b_0^{n_2}b_1b_0^m b_1b_0^{n_1} \equiv\ & b_2b_0^{n_3}b_1b_0^{n_2}b_1b_0^m b_1b_0^{n_1} + b_1b_0^{n_3}b_2b_0^{n_2}b_1b_0^m b_1b_0^{n_1} \\ & + b_1b_0^{n_3}b_1b_0^{n_2}b_2b_0^m b_1b_0^{n_1} + b_1b_0^{n_3}b_1b_0^{n_2}b_1b_0^m b_2b_0^{n_1} \\ & \mod \text{ words } w \text{ satisfying } b(w) = 0, \\ b_1 *_q b_1b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1}b_1b_0^m \equiv\ & b_2b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1}b_1b_0^m + b_1b_0^{n_3}b_2b_0^{n_2}b_1b_0^{n_1}b_1b_0^m \\ & + b_1b_0^{n_3}b_1b_0^{n_2}b_2b_0^{n_1}b_1b_0^m + b_1b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1}b_2b_0^m \\ & \mod \text{ words } w \text{ satisfying } b(w) = 0. \end{aligned}$$

Therefore, we deduce by applying the τ-invariance of the balanced multiple q-zeta values

$$\begin{aligned} & \zeta_q(b_{n_1+1}b_{n_2+1}b_{n_3+1}b_{m+1}b_0) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{n_3+1}b_0b_{m+1}) + \zeta_q(b_{n_1+1}b_{n_2+1}b_0b_{n_3+1}b_{m+1}) \\ & + \zeta_q(b_{n_1+1}b_0b_{n_2+1}b_{n_3+1}b_{m+1}) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{m+1}b_{n_3+1}b_0) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{m+1}b_0b_{n_3+1}) \\ & + \zeta_q(b_{n_1+1}b_{n_2+1}b_0b_{m+1}b_{n_3+1}) + \zeta_q(b_{n_1+1}b_0b_{n_2+1}b_{m+1}b_{n_3+1}) + \zeta_q(b_{n_1+1}b_{m+1}b_{n_2+1}b_{n_3+1}b_0) \\ & + \zeta_q(b_{n_1+1}b_{m+1}b_{n_2+1}b_0b_{n_3+1}) + \zeta_q(b_{n_1+1}b_{m+1}b_0b_{n_2+1}b_{n_3+1}) + \zeta_q(b_{n_1+1}b_0b_{m+1}b_{n_2+1}b_{n_3+1}) \\ & + \zeta_q(b_{m+1}b_{n_1+1}b_{n_2+1}b_{n_3+1}b_0) + \zeta_q(b_{n_1+1}b_{m+1}b_{n_2+1}b_0b_{n_3+1}) + \zeta_q(b_{n_1+1}b_{m+1}b_0b_{n_2+1}b_{n_3+1}) \\ & + \zeta_q(b_{n_1+1}b_0b_{m+1}b_{n_2+1}b_{n_3+1}) \quad \in \mathcal{Z}_q^\circ. \end{aligned} \tag{6.5.8}$$

Subtracting (6.5.7) from (6.5.8), we obtain

$$\begin{aligned}&\zeta_q(b_{n_1+1}b_0b_{n_2+1}b_{n_3+1}b_{m+1}) + \zeta_q(b_{n_1+1}b_0b_{n_2+1}b_{m+1}b_{n_3+1}) + \zeta_q(b_{n_1+1}b_0b_{m+1}b_{n_2+1}b_{n_3+1})\\ &+ \zeta_q(b_{n_1+1}b_{n_2+1}b_0b_{n_3+1}b_{m+1}) + \zeta_q(b_{n_1+1}b_{n_2+1}b_0b_{m+1}b_{n_3+1}) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{n_3+1}b_0b_{m+1})\\ &\in \mathcal{Z}_q^\circ.\end{aligned}$$

Applying the results from the first case (6.5.3) and the second case (6.5.6), we deduce

$$\zeta_q(b_{n_1+1}b_{n_2+1}b_{n_3+1}b_0b_{m+1}) \in \mathcal{Z}_q^\circ. \tag{6.5.9}$$

Finally, let $n_1, n_2, n_4, n_4 \geq 0$. We calculate

$$\begin{aligned}b_1 *_q b_1b_0^{n_4}b_1b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1} \equiv\ & b_2b_0^{n_4}b_1b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1} + b_1b_0^{n_4}b_2b_0^{n_3}b_1b_0^{n_2}b_1b_0^{n_1}\\ &+ b_1b_0^{n_4}b_1b_0^{n_3}b_2b_0^{n_2}b_1b_0^{n_1} + b_1b_0^{n_4}b_1b_0^{n_3}b_1b_0^{n_2}b_2b_0^{n_1}\\ &\mod \text{ words } w \text{ satisfying } b(w) = 0.\end{aligned}$$

Thus by applying the τ-invariance of the balanced multiple q-zeta values, we deduce

$$\begin{aligned}&\zeta_q(b_{n_1+1}b_{n_2+1}b_{n_3+1}b_{n_4+1}b_0) + \zeta_q(b_{n_1+1}b_{n_2+1}b_{n_3+1}b_0b_{n_4+1}) + \zeta_q(b_{n_1+1}b_{n_2+1}b_0b_{n_3+1}b_{n_4+1})\\ &+ \zeta_q(b_{n_1+1}b_0b_{n_2+1}b_{n_3+1}b_{n_4+1}) \quad \in \mathcal{Z}_q^\circ.\end{aligned}$$

Together with the results in the previous cases (6.5.3), (6.5.6), and (6.5.9), this shows

$$\zeta_q(b_{n_1+1}b_{n_2+1}b_{n_3+1}b_{n_4+1}b_0) \in \mathcal{Z}_q^\circ.$$

Appendix A Introduction to the algebraic framework

This section provides an introduction to Hopf algebras, quasi-shuffle algebras, and affine group schemes. In the following, let R be a commutative $\mathbb{Q}$-algebra with unit. Note that we assume any algebra to be associative by definition.

A.1 Graded algebras

We introduce graded algebras and their Hilbert-Poincare series. Proofs for the provided results are given in [Bou89], [Foi], [Ok15], or [Re93].

Definition A.1. An R-module M is graded if there is a family $(M^{(i)})_{i\geq 0}$ of free submodules of M of finite rank, such that

$$M = \bigoplus_{i\geq 0} M^{(i)}.$$

The elements in $M^{(i)}$ are called homogeneous of degree i. Moreover, the Hilbert-Poincare series of M is given by

$$H_M(x) = \sum_{i\geq 0} \operatorname{rank}_R(M^{(i)})x^i.$$

Lemma A.2. *Let M, N be graded R-modules. Then also the R-modules $M \oplus N$ and $M \otimes N$ are graded via*

$$(M \oplus N)^{(i)} = M^{(i)} \oplus N^{(i)}, \qquad (M \otimes N)^{(i)} = \bigoplus_{a+b=i} M^{(a)} \otimes N^{(b)}.$$

In this case, the following holds

$$H_{M\oplus N}(x) = H_M(x) + H_N(x), \qquad H_{M\otimes N}(x) = H_N(x)H_M(x).$$

□

Definition A.3. A unitary R-algebra $(A, \cdot, 1)$ is graded, if $A = \bigoplus_{i\geq 0} A^{(i)}$ is a graded R-module and

$$A^{(i)} \cdot A^{(j)} \subset A^{(i+j)}.$$

If $(A, \cdot, 1)$ is a graded algebra, then $1 \in A^{(0)}$.

Example A.4. Let $M = \bigoplus_{i\geq 0} M^{(i)}$ be a graded R-module and $M^{(0)} = \{0\}$. Then the tensor algebra $\mathcal{T}(M) = \bigoplus_{n\geq 0} M^{\otimes n}$ (with $M^{\otimes 0} = R$) is graded via

$$\mathcal{T}(M)^{(0)} = R, \qquad \mathcal{T}(M)^{(i)} = (M^{\otimes 1})^{(i)} \oplus \cdots \oplus (M^{\otimes i})^{(i)}, \ i \geq 1.$$

Proposition A.5. *Let $(A, \cdot, 1)$ be a unitary, commutative, free, graded R-algebra satisfying* $\operatorname{rank} A^{(0)} = 1$. *Then, one has*

$$H_A(x) = \prod_{i\geq 1} (1 - x^i)^{-g_i},$$

where g_i denotes the number of algebra generators of A of degree i. □

Definition A.6. Let M be an R-module. Then the symmetric algebra of M is given by $\mathcal{S}(M) = {}^{\mathcal{T}(M)}\!/_{J}$, where J is the ideal generated by the elements $m_1 \otimes m_2 - m_2 \otimes m_1$ for all $m_1, m_2 \in M$.

For example, if M is a free R-module of rank r, then one obtains $\mathcal{S}(M) \simeq R[x_1, \dots, x_r]$.

Let $M = \bigoplus_{i\geq 0} M^{(i)}$ be a graded R-module and $M^{(0)} = \{0\}$. Then the ideal J in Definition A.6 is graded, i.e., one has

$$J = \bigoplus_{i\geq 0} J^{(i)} = \bigoplus_{i\geq 0} \mathcal{T}(M)^{(i)} \cap J,$$

and hence also $\mathcal{S}(M)$ is graded via

$$\mathcal{S}(M)^{(i)} = {\mathcal{T}(M)^{(i)}}\big/{J^{(i)}}.$$

The symmetric algebra $\mathcal{S}(M)$ is a commutative, free R-algebra generated by a basis of M, thus Proposition A.5 implies the following.

Corollary A.7. *Let $M = \bigoplus_{i\geq 0} M^{(i)}$ be a graded R-module and $M^{(0)} = \{0\}$. Then the Hilbert-Poincare series of $\mathcal{S}(M)$ is given by*

$$H_{\mathcal{S}(M)}(x) = \prod_{i\geq 1} (1 - x^i)^{\mathrm{rank}_R(M^{(i)})}.$$

Next, we want to investigate non-commutative graded algebras.

Proposition A.8. *If $(A, \cdot, 1)$ is a unitary, non-commutative, free, graded R-algebra over some countable set $\mathcal{Z}$, then the following holds*

$$H_A(x) = \big(1 - \sum_{z\in\mathcal{Z}} x^{\deg(z)}\big)^{-1}.$$

□

An important class of non-commutative algebras is given by the following.

Definition A.9. A Lie algebra over R is an R-module L equipped with an R-linear map

$$[\cdot,\cdot] : L \otimes L \to L,$$

such that the following holds for all $x, y, z \in L$

(i) Anti symmetry: $[x, x] = 0$,

(ii) Jacobi's identity: $[[x, y], z] + [[y, z], x] + [[z, x], y] = 0$.

The map $[\cdot,\cdot]$ is called the Lie bracket.

A Lie algebra $(L, [\cdot,\cdot])$ is graded, if $L = \bigoplus_{i\geq 0} L^{(i)}$ is a graded R-module and one has for all $i, j \geq 0$

$$[L^{(i)}, L^{(j)}] \subset L^{(i+j)}.$$

Example A.10. Let $(A, \cdot, 1)$ be an R-algebra and define the commutator bracket by

$$[a, b] = a \cdot b - b \cdot a, \qquad a, b \in A.$$

Then the pair $(A, [-,-])$ is a Lie algebra over R.

Definition A.11. Let $(L, [\cdot,\cdot])$ be a Lie algebra over R. Then the universal enveloping algebra of L is given by $\mathcal{U}(L) = {\mathcal{T}(L)}\big/{K}$, where K is the ideal generated by the elements $x \otimes y - y \otimes x - [x, y]$ for all $x, y \in L$.

Let $(L, [\cdot,\cdot])$ be a graded Lie algebra over R and $L^{(0)} = \{0\}$. Then the ideal K in Definition A.11 is a graded ideal, and thus also the universal enveloping algebra $\mathcal{U}(L)$ is graded via

$$\mathcal{U}(L)^{(i)} = {\mathcal{T}(V)^{(i)}}\big/{K^{(i)}}.$$

Assume that the generators in the Lie algebra L only satisfy independent relations. Since $\mathcal{U}(L)$ is a non-commutative R-algebra, Proposition A.8 implies

$$H_{\mathcal{U}(L)}(x) = (1 - \sum_{i\geq 0} g_i x^i + \sum_{i\geq 0} r_i x^i)^{-1}, \tag{A.11.1}$$

where g_i denotes the number of algebra generators of $L^{(i)}$ and r_i denotes the number of independent relations in $L^{(i)}$.

At the end of this subsection, we will explain how to obtain a basis for some free Lie algebra and hence also its universal enveloping algebra and symmetric algebra. Clearly, the number of basis elements yields a formula for the Hilbert-Poincare series.

Definition A.12. Let $\mathcal{A}$ be an ordered set. Denote by $(R\langle\mathcal{A}\rangle, \mathrm{conc}, \mathbf{1})$ the free non-commutative algebra over R generated by $\mathcal{A}$ and call the monic monomials in $R\langle\mathcal{A}\rangle$ words. Extend the ordering lexicographically to all words in $R\langle\mathcal{A}\rangle$.

(i) A word $w \in R\langle\mathcal{A}\rangle\backslash R\mathbf{1}$ is called a Lyndon word if for every nontrivial decomposition $w = uv$ one obtains $w < v$.

(ii) For a Lyndon word $w \in R\langle\mathcal{A}\rangle$ the standard bracket $\gamma(w)$ contained in the free Lie algebra $\mathrm{Lie}_R\langle\mathcal{A}\rangle$ generated by $\mathcal{A}$ is recursively defined as

- If $w \in \mathcal{A}$, then set $\gamma(w) = w$.
- If w consists at least of two elements in $\mathcal{A}$, then write $w = uv$ with u, v Lyndon words and v as long as possible and set $\gamma(w) = [\gamma(u), \gamma(v)]$.

As a special case of [Re93, Theorem 4.9 (i)] the following holds.

Theorem A.13. *Let $L = \mathrm{Lie}_R\langle\mathcal{A}\rangle$ be a free Lie algebra generated by some ordered set $\mathcal{A}$. Then the set of all standard brackets is a basis for L.* □

Example A.14. Let $L = \mathrm{Lie}_R\langle f_1, f_2, \ldots\rangle$ be the free Lie algebra over R generated by $f_1, f_2, \ldots$. Set $\deg(f_i) = i$ and extend this to a grading on L, i.e., set

$$\deg(f_{i_1} \ldots f_{i_n}) = i_1 + \cdots + i_n.$$

The universal enveloping algebra of L is the free non-commutative algebra generated by $f_1, f_2, \ldots$, so $\mathcal{U}(L) = R\langle f_1, f_2, \ldots\rangle$. The algebra $\mathcal{U}(L)$ inherits the grading of L and thus one obtains from Proposition A.8

$$H_{\mathcal{U}(L)}(x) = \frac{1}{1 - x - x^2 - x^3 - \ldots}.$$

We also want to compute the Hilbert-Poincare series of the symmetric algebra $\mathcal{S}(L)$, since this algebra also inherits the grading from L. It is well-known that the symmetric algebra is a free polynomial algebra in any basis of L, thus we have to determine a basis of L. According to Definition A.12, we have to compute the Lyndon words (with respect to the ordering $f_i < f_j$ iff $i < j$). For example, the Lyndon words of degree ≤ 6 are given by

$f_1,\ f_2,\ f_3,\ f_1f_2,\ f_4,\ f_1f_3,\ f_1f_1f_2,\ f_5,\ f_1f_4,\ f_2f_3,\ f_1f_1f_3,\ f_1f_2f_2,$
$f_1f_1f_1f_2,\ f_6,\ f_1f_5,\ f_2f_4,\ f_1f_1f_4,\ f_1f_2f_3,\ f_1f_3f_2,\ f_1f_1f_1f_3,\ f_1f_1f_2f_2,$
$f_1f_1f_1f_1f_2.$

and the corresponding standard brackets are

$$f_1, \quad f_2, \quad f_3, \quad [f_1,f_2], \quad f_4, \quad [f_1,f_3], \quad [f_1,[f_1,f_2]], \quad f_5, \quad [f_1,f_4], \quad [f_2,f_3],$$
$$[f_1,[f_1,f_3]], \quad [[f_1,f_2],f_2], \quad [f_1,[f_1,[f_1,f_2]]], \quad f_6, \quad [f_1,f_5], \quad [f_2,f_4], \quad [f_1,[f_1,f_4]],$$
$$[f_1,[f_2,f_3]], \quad [[f_1,f_3],f_2], \quad [f_1,[f_1,[f_1,f_3]]], \quad [f_1,[[f_1,f_2],f_2]], \quad [f_1,[f_1,[f_1,[f_1,f_2]]]].$$

By Theorem A.13 the standard brackets form a basis of L. Thus by Proposition A.5, we have to count the number of standard brackets (or equivalently the number of Lyndon words) to obtain the Hilbert-Poincare series of the symmetric algebra $\mathcal{S}(L)$. This gives

$$H_{\mathcal{S}(L)}(x) = (1-x)(1-x^2)(1-x^3)^2(1-x^4)^3(1-x^5)^6(1-x^6)^9 \ldots.$$

Actually applying Möbius inversion, one obtains an explicit formula for the number $N(d)$ of Lyndon words in degree d (cf [Re93, Corollary 4.14]) and then gets

$$H_{\mathcal{S}(L)}(x) = \prod_{d \geq 1} (1-x^d)^{N(d)}.$$

A.2 Hopf algebras

This subsection gives an introduction to Hopf algebras. We start by introducing algebras and coalgebras as dual structures. Then we will provide the notion of bialgebras and Hopf algebras. In particular, we will define the set of grouplike elements, primitive elements, and indecomposables and present their additional structures and relations between them. We will end by introducing the concept of completion of Hopf algebras. All presented results can be found in [AB80], [Ca07], [Foi], [Man08], or [MM65].

Algebras. We will reformulate the usual definitions for algebras in terms of linear maps to motivate the definition of coalgebras.

Let $(A,\cdot,1)$ be a unitary R-algebra. Then the product $\cdot$ can be considered as an R-linear map

$$m: A \otimes A \to A, \quad a_1 \otimes a_2 \mapsto a_1 \cdot a_2.$$

Then associativity is equivalent to requiring that the following diagram commutes

$$\begin{array}{ccc} A \otimes A \otimes A & \xrightarrow{m \otimes \mathrm{id}} & A \otimes A \\ {\scriptstyle \mathrm{id} \otimes m}\downarrow & & \downarrow{\scriptstyle m} \\ A \otimes A & \xrightarrow{\quad m \quad} & A \end{array}.$$

Similarly, the unit 1 can be considered as an R-linear map

$$\eta: R \to A, \quad \lambda \mapsto \lambda 1.$$

Then the axiom of a unit is given by the commutativity of the following diagram

$$\begin{array}{ccccc} R \otimes A & \xrightarrow{\eta \otimes \mathrm{id}} & A \otimes A & \xleftarrow{\mathrm{id} \otimes \eta} & A \otimes R \\ & {\scriptstyle \mathrm{id}}\searrow & \downarrow{\scriptstyle m} & \swarrow{\scriptstyle \mathrm{id}} & \\ & & A & & \end{array}.$$

In this diagram, the following canonical isomorphisms of tensor products are used

$$R \otimes A \xrightarrow{\sim} A \xrightarrow{\sim} A \otimes R,$$
$$\lambda \otimes a \mapsto \lambda a \mapsto a \otimes \lambda.$$

A submodule $B \subset A$ is a subalgebra of A if $m(B \otimes B) \subset B$ and $\eta(R) \subset B$. Similarly, a submodule $I \subset A$ is an algebra ideal if $m(A \otimes I + I \otimes A) \subset I$.

Define the R-linear map

$$t : A \otimes A \to A \otimes A, \qquad a_1 \otimes a_2 \mapsto a_2 \otimes a_1. \tag{A.14.1}$$

Then an R-algebra (A, m, η) is commutative if $m \circ t = m$.

An R-algebra A is graded if $A = \bigoplus_{i \geq 0} A^{(i)}$ is a graded R-module (Definition A.1) and

$$m(A^{(i)} \otimes A^{(j)}) \subseteq A^{(i+j)}, \qquad i, j \geq 0.$$

In this case, one has $\eta(R) \subseteq A^{(0)}$.

The axioms of an algebra morphism $\Phi : (A, m, \eta) \to (A', m', \eta')$ can be rephrased as commutativity of the following diagrams

$$\begin{array}{ccc} A \otimes A & \xrightarrow{\Phi \otimes \Phi} & A' \otimes A' \\ \downarrow{\scriptstyle m} & & \downarrow{\scriptstyle m'} \\ A & \xrightarrow{\quad\Phi\quad} & A' \end{array}, \qquad \begin{array}{ccc} R & \xrightarrow{\eta} & A \\ & \searrow^{\eta'} & \downarrow{\scriptstyle \Phi} \\ & & A' \end{array}.$$

Lemma A.15. *Let (A, m, η) be an R-algebra. Then the tensor product $A \otimes A$ equipped with the maps*

$$\begin{aligned} m_\otimes &: (A \otimes A) \otimes (A \otimes A) \to A \otimes A, \\ &\quad (a_1 \otimes a_1') \otimes (a_2 \otimes a_2') \mapsto m(a_1 \otimes a_2) \otimes m(a_1' \otimes a_2'), \\ \eta_\otimes &: R \to A \otimes A, \\ &\quad \lambda \mapsto \lambda(\eta(1) \otimes \eta(1)) \end{aligned}$$

is again an R-algebra. □

In the following, we will use both notions for an algebra, either we give the product and the unit directly or we define the product and unit maps.

Coalgebras. By reversing the arrows in the previously given new description of algebras, we obtain the concept of coalgebras.

Definition A.16. An R-module C equipped with two R-linear maps

$$\begin{aligned} \Delta &: C \to C \otimes C, \\ \varepsilon &: C \to R, \end{aligned}$$

is called a coalgebra if the following diagrams commute

$$\begin{array}{ccc} C & \xrightarrow{\quad\Delta\quad} & C \otimes C \\ {\scriptstyle \Delta}\downarrow & & \downarrow{\scriptstyle \mathrm{id} \otimes \Delta} \\ C \otimes C & \xrightarrow{\Delta \otimes \mathrm{id}} & C \otimes C \otimes C \end{array} \qquad \text{(coassociativity)},$$

$$\begin{array}{ccccc} R \otimes C & \xleftarrow{\varepsilon \otimes \mathrm{id}} & C \otimes C & \xrightarrow{\mathrm{id} \otimes \varepsilon} & C \otimes R \\ & {\scriptstyle \mathrm{id}}\nwarrow & {\scriptstyle \Delta}\uparrow & \nearrow{\scriptstyle \mathrm{id}} & \\ & & C & & \end{array} \qquad \text{(counitarity)}.$$

A submodule $D \subset C$ is a subcoalgebra if $\Delta(D) \subset D \otimes D$. Similarly, $I \subset C$ is a coideal if $\Delta(I) \subset I \otimes C + C \otimes I$ and $\varepsilon(I) = \{0\}$.

An R-coalgebra (C, Δ, ε) is cocommutative if $t \circ \Delta = \Delta$, where t permutes the tensor product factors (see (A.14.1)).

An R-coalgebra (C, Δ, ε) is graded, if $C = \bigoplus_{i \geq 0} C^{(i)}$ is a graded R-module (Definition A.1) and

$$\Delta(C^{(i)}) \subseteq \sum_{m+n=i} C^{(m)} \otimes C^{(n)}, \qquad i \geq 0.$$

One has then $\varepsilon(C^{(i)}) = \{0\}$ for each $i \geq 1$.

An R-coalgebra morphism is an R-linear map $\Phi : (C, \Delta, \varepsilon) \to (C', \Delta', \varepsilon')$, such that the following diagrams commute

$$\begin{array}{ccc} C & \xrightarrow{\Phi} & C' \\ {\scriptstyle \Delta}\downarrow & & \downarrow{\scriptstyle \Delta'} \\ C \otimes C & \xrightarrow{\Phi \otimes \Phi} & C' \otimes C' \end{array}, \qquad \begin{array}{ccc} C & \xrightarrow{\varepsilon} & R \\ {\scriptstyle \Phi}\downarrow & \nearrow_{\varepsilon'} & \\ C' & & \end{array}.$$

The tensor product of coalgebras can also be equipped with a coalgebra structure.

Lemma A.17. *Let (C, Δ, ε) be an R-coalgebra. Then the tensor product $C \otimes C$ together with the maps*

$$\begin{aligned} \Delta_\otimes &: C \otimes C \to (C \otimes C) \otimes (C \otimes C), \\ &\quad (c_1 \otimes c_2) \mapsto (\mathrm{id} \otimes t \otimes \mathrm{id})(\Delta(c_1) \otimes \Delta(c_2)), \\ \varepsilon_\otimes &: C \otimes C \to R, \\ &\quad c_1 \otimes c_2 \mapsto \varepsilon(c_1)\varepsilon(c_2), \end{aligned}$$

is also an R-coalgebra. □

Duality. We will introduce the concept of dual modules and dual graded modules with respect to a pairing and explain dual maps. We will see that the structures of algebras and coalgebras are dual in this sense. Moreover, we will obtain the dual structure of Lie algebras.

Definition A.18. Two R-modules M and N are dual, if there is an R-linear map

$$(\cdot \mid \cdot) : M \otimes N \to R,$$

such that

(i) if $(m \mid n) = 0$ for all $n \in N$, then $m = 0$,
(ii) if $(m \mid n) = 0$ for all $m \in M$, then $n = 0$.

In this case, $(\cdot \mid \cdot)$ is called the duality pairing of M and N.

Let M and N be graded R-modules. If there is a duality pairing $(\cdot \mid \cdot) : M \otimes N \to R$, such that

$$(M^{(i)} \mid N^{(j)}) = 0 \quad \text{for all } i \neq j,$$

then M and N are graded dual. In this case, we say that $(\cdot \mid \cdot)$ is a graded duality pairing.

Example A.19. (i) Let M be a free R-module of finite rank. Then the usual dual module is defined by

$$M^* = \mathrm{Hom}_{R\text{-lin}}(M, R).$$

The modules M and M^* are dual in the sense of Definition A.18, the duality pairing is given by

$$\begin{aligned}(\cdot \mid \cdot) : M^* \otimes M &\to R,\\ f \otimes m &\mapsto f(m).\end{aligned}$$

(ii) Let M be a graded R-module (Definition A.1). Then its usual graded dual is defined by

$$M^\vee = \bigoplus_{i \geq 0} (M^{(i)})^*.$$

The modules M and $M^\vee$ are also graded dual in the sense of Definition A.18, the graded duality pairing is given by

$$\begin{aligned}&M^\vee \otimes M \to R,\\ &f_i \otimes m_j \mapsto \begin{cases} f_i(m_j), & i = j,\\ 0 & \text{else}\end{cases} \qquad (\text{where } f_i \in (M^{(i)})^*,\ m_j \in M^{(j)}).\end{aligned}$$

Proposition A.20. *(i) Let M, N be dual free R-modules of finite rank. Then one has*

$$\mathrm{rank}_R(M) = \mathrm{rank}_R(N).$$

(ii) Let M, N be graded dual R-modules. Then for each $i \geq 0$, the following holds

$$\mathrm{rank}_R(M^{(i)}) = \mathrm{rank}_R(N^{(i)}).$$

□

Definition A.21. Let M_1, N_1 be dual R-modules for the pairing $(\cdot \mid \cdot)_1$, M_2, N_2 be dual R-modules for the pairing $(\cdot \mid \cdot)_2$ and $f : M_1 \to M_2$ be an R-linear map. The dual map to f is the unique R-linear map $g : N_2 \to N_1$ satisfying

$$(f(m), n)_2 = (m, g(n))_1 \qquad \text{for all } m \in M_1,\ n \in N_2.$$

Lemma A.22. *Let M, N be (graded) dual R-modules for the pairing $(\cdot \mid \cdot)$. Then also $M \otimes M$ and $N \otimes N$ are (graded) dual R-modules, the (graded) duality pairing is given by*

$$(m_1 \otimes m_2 \mid n_1 \otimes n_2)_\otimes = (m_1 \mid n_1)(m_2 \mid n_2)$$

for all $m_1, m_2 \in M$ and $n_1, n_2 \in N$. □

Theorem A.23. *(i) Let (A, m, η) be a (graded) R-algebra. If C is an R-module (graded) dual to A, then C equipped with the dual maps of m and η is a (graded) R-coalgebra.*

(ii) Let (C, Δ, ε) be a (graded) R-coalgebra. If A is an R-module (graded) dual to C, then A together with the dual maps of Δ and ε is a (graded) R-algebra. □

There is also a dual notion for Lie algebras (Definition A.9).

Definition A.24. A Lie coalgebra over R is an R-module E equipped with an R-linear map

$$\delta : E \to E \otimes E,$$

such that

(i) Anti symmetry: $t \circ \delta = -\delta$

(ii) Cocycle condition: $(\delta \otimes \mathrm{id}) \circ \delta = (\mathrm{id} \otimes \delta) \circ \delta + (\mathrm{id} \otimes t) \circ (\delta \otimes \mathrm{id}) \circ \delta$

The map δ is called the Lie cobracket of E. Moreover, the map t is given in (A.14.1).

Proposition A.25. *(i) Let $(L, [-,-])$ be a Lie algebra over R. If E is an R-module (graded) dual to the module L, then E equipped with the dual map of the Lie bracket $[-,-]$ is a Lie coalgebra over R.*

(ii) Let (E, d) be a Lie coalgebra over R. If L is a graded dual R-module to E, then L equipped with the dual map of d is a Lie algebra over R. □

Bialgebras. We are interested in modules, which are equipped with the structure of an algebra and a coalgebra at the same time and satisfy certain compatibility conditions. This leads to the notion of bialgebras.

Definition A.26. If an R-module B is equipped with an algebra structure (B, m, η) and a coalgebra structure (B, Δ, ε), such that the maps Δ and ε are algebra morphisms (or equivalently, such that m and η are coalgebra morphisms), then $(B, m, \eta, \Delta, \varepsilon)$ is called an R-bialgebra.

The algebra and coalgebra structure on $B \otimes B$ is explained in Lemma A.15, A.17.

A submodule $B' \subset B$ is a subbialgebra if B' is a subalgebra and a subcoalgebra. Similarly, a submodule $I \subset B$ is a biideal if it is an algebra ideal and a coalgebra ideal.

An R-bialgebra $(B, m, \eta, \Delta, \varepsilon)$ is graded if it is graded as an algebra and as a coalgebra.

An R-bialgebra morphism is an R-linear map $\Phi : (B, m, \eta, \Delta, \varepsilon) \to (B', m', \eta', \Delta', \varepsilon')$, which is simultaneously an algebra and a coalgebra morphism.

Theorem A.27. *Let $(B, m, \eta, \Delta, \varepsilon)$ be a (graded) R-bialgebra. If B' is an R-module (graded) dual to B, then B' equipped with the dual maps of m, η, Δ and ε is also a (graded) R-bialgebra.* □

Proposition A.28. *Let $(B, m, \eta, \Delta, \varepsilon)$ be an R-bialgebra. Then $\mathrm{Hom}_{R\text{-lin}}(B, B)$ equipped with the product*

$$f \star g = m \circ (f \otimes g) \circ \Delta$$

and the unit

$$i : B \to B, \ b \mapsto \varepsilon(b)\eta(1)$$

is an R-algebra. This algebra is called the convolution algebra of H. □

Hopf algebras. With the previously given background, we are able to define Hopf algebras. Those are a subclass of the bialgebras with particularly nice behavior.

Definition A.29. A Hopf algebra over R is a bialgebra $(H, m, \eta, \Delta, \varepsilon)$, where the identity admits an inverse S in the convolution algebra $(\mathrm{Hom}_{R\text{-lin}}(H, H), \star, i)$ (given in Proposition A.28). The inverse S is called the antipode.

A submodule $H' \subset H$ is a Hopf subalgebra if H' is a subbialgebra and $S(H') \subset H'$. Similarly, $I \subset H$ is a Hopf ideal if I is a biideal and $S(I) \subset I$.

A Hopf algebra $(H, m, \eta, \Delta, \varepsilon)$ over R is graded, if it is graded as a bialgebra and

$$S(H^{(i)}) \subseteq H^{(i)}, \qquad i \geq 0.$$

In the following, we sometimes just give the product and coproduct map for a Hopf algebra, since the other maps are often clear from the context. The same also applies to algebras, coalgebras, and bialgebras.

Proposition A.30. *Let $(H, m, \eta, \Delta, \varepsilon, S)$ and $(H', m', \eta', \Delta', \varepsilon', S')$ be Hopf algebras over R. Then for any R-bialgebra morphism $\Phi : (H, m, \eta, \Delta, \varepsilon) \to (H', m', \eta', \Delta', \varepsilon')$, one has*

$$S' \circ \Phi = \Phi \circ S.$$

□

Due to the previous proposition, a Hopf algebra morphism is simply defined to be a bialgebra morphism.

Theorem A.31. *Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a (graded) Hopf algebra over R. If H' is an R-module (graded) dual to H, then H' equipped with the dual maps of m, η, Δ, ε and S is also a (graded) Hopf algebra over R.* □

Proposition A.32. *Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a Hopf algebra over R. Then the antipode S is an anti-morphism, i.e., the following holds*

$$S \circ m = m \circ t \circ (S \otimes S).$$ □

Recall that t simply permutes the tensor product factors (see (A.14.1)).

Theorem A.33. *Let $(B, m, \eta, \Delta, \varepsilon)$ be a graded R-bialgebra. If B is connected, i.e., one has* $\operatorname{rank}_R B^{(0)} = 1$*, then B is a Hopf algebra over R.* □

Example A.34. (i) Let M be a graded R-module with $M^{(0)} = \{0\}$. The tensor algebra $\mathcal{T}(M)$ (Example A.4) equipped with the coproduct $\Delta_{\sqcup\!\sqcup}(m) = 1 \otimes m + m \otimes 1$ and the antipode $S(m) = -m$ for all $m \in M$ is a graded, cocommutative Hopf algebra over R. Note that $\Delta_{\sqcup\!\sqcup}$ is an algebra morphism and S is an algebra anti morphism, so both maps are determined uniquely by its images on M.

(ii) Consider the symmetric algebra $\mathcal{S}(M) = {}^{\mathcal{T}(M)}\!/_{J}$ (Definition A.6). Since J is a Hopf ideal of $\mathcal{T}(M)$, the symmetric algebra $\mathcal{S}(M)$ is a graded, commutative, and cocommutative Hopf algebra.

(iii) Let $(L, [\cdot, \cdot])$ be a graded Lie algebra over R with $L^{(0)} = \{0\}$ and consider the universal enveloping algebra $\mathcal{U}(L) = {}^{\mathcal{T}(L)}\!/_{K}$ (Definition A.11). Since K is also a Hopf ideal, the universal enveloping algebra $\mathcal{U}(L)$ is a graded, cocommutative Hopf algebra.

Proposition A.35. *Let L be a graded Lie algebra over R and $L^{(0)} = \{0\}$. Then there is an algebra isomorphism*

$$\mathcal{U}(L)^\vee \simeq \mathcal{S}(L^\vee).$$

□

The usual graded duals $L^\vee$ and $\mathcal{U}(L)^\vee$ are defined in Example A.19 (ii). Proposition A.20 implies the following for the corresponding Hilbert-Poincare series.

Corollary A.36. *For any graded Lie algebra $(L, [\cdot, \cdot])$ over R satisfying $L^{(0)} = \{0\}$, one has*

$$H_{\mathcal{S}(L)}(x) = H_{\mathcal{U}(L)}(x).$$

So by Corollary A.7 and (A.11.1), one obtains two different expressions of the Hilbert-Poincare series of a symmetric algebra or universal enveloping algebra.

Definition A.37. Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a Hopf algebra over R. An element $x \in H \backslash \{0\}$ is called grouplike if

$$\Delta(x) = x \otimes x.$$

The set of grouplike elements in H is denoted by $\mathrm{Grp}(H)$. An element $x \in H$ is called primitive if it satisfies

$$\Delta(x) = 1 \otimes x + x \otimes 1.$$

By $\mathrm{Prim}(H)$ we denote the set of all primitive elements in H.

Theorem A.38. *Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a Hopf algebra over R.*

(i) The set $\mathrm{Grp}(H)$ equipped with the product and the unit of H forms a group. For an element $x \in \mathrm{Grp}(H)$, the inverse element is given by $S(x)$. Moreover, each grouplike element $x \in H$ satisfies $\varepsilon(x) = 1$.

(ii) The set $\mathrm{Prim}(H)$ equipped with the commutator bracket $[x, y] = m(x \otimes y) - m(y \otimes x)$ is a Lie algebra. Furthermore, one has for each primitive element $x \in H$ that $\varepsilon(x) = 0$ and $S(x) = -x$. □

Theorem A.39. *(Cartier-Quillen-Milnor-Moore) Let H be a graded cocommutative Hopf algebra over R, such that $\operatorname{rank} H_R^{(0)} = 1$. Then there is a Hopf algebra isomorphism*

$$H \simeq \mathcal{U}(\mathrm{Prim}(H)).$$ □

Corollary A.40. *Let $(R\langle\mathcal{A}\rangle, \mathrm{conc}, \mathbf{1})$ be the non-commutative free algebra over R generated by the set $\mathcal{A}$. Define the coproduct $\Delta_{\sqcup\!\sqcup}$ by $\Delta_{\sqcup\!\sqcup}(a) = a \otimes \mathbf{1} + \mathbf{1} \otimes a$ for all $a \in \mathcal{A}$ (and extend this with respect to concatenation), then $(R\langle\mathcal{A}\rangle, \mathrm{conc}, \Delta_{\sqcup\!\sqcup})$ is a cocommutative Hopf algebra. One has*

$$\mathrm{Prim}(R\langle\mathcal{A}\rangle) = \mathrm{Lie}_R\langle\mathcal{A}\rangle.$$ □

Definition A.41. Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a Hopf algebra over R. The space of indecomposables of H is defined as

$$\mathrm{Q}(H) = {}^{\ker(\varepsilon)}\!\big/_{\ker(\varepsilon)^2}.$$

If $(H, m, \eta, \Delta, \varepsilon, S)$ is a graded algebra with $H = \bigoplus_{i \geq 0} H^{(i)}$, then from the observations on p. 157 one obtains

$$\ker(\varepsilon) = \bigoplus_{i \geq 1} H^{(i)}.$$

Let (C, Δ, ε) be an R-coalgebra. Then define a corresponding Lie cobracket δ to Δ by

$$\delta = (\mathrm{id} - t) \circ \Delta : C \to C \otimes C, \tag{A.41.1}$$

where t simply permutes the tensor product functors (see (A.14.1)).

Proposition A.42. *Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a Hopf algebra over R. Then the corresponding Lie cobracket to Δ defined in (A.41.1) induces a Lie coalgebra structure on the space $\mathrm{Q}(H)$ of indecomposables.* □

This Lie coalgebra structure is closely related to the Lie algebra structure on the primitive elements (Theorem A.38 (ii)).

Theorem A.43. *([MM65, Proposition 3.10]) Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a graded Hopf algebra over R. Then there is an isomorphism of Lie algebras over R*

$$\mathrm{Prim}(H^\vee) \simeq \mathrm{Q}(H)^\vee.$$ □

The usual graded duals $H^\vee$ and $\mathrm{Q}(H)^\vee$ are defined in Example A.19 (ii).

Completed Hopf algebras and the exponential map. We will introduce the concept of completions with respect to a filtration. This will lead to the notion of completed Hopf algebras, for which we will obtain a bijection between the grouplike and primitive elements.

Definition A.44. (i) Let M be an R-module equipped with a descending filtration, i.e., there is a chain of submodules

$$M = \operatorname{Fil}^{(0)} M \supset \operatorname{Fil}^{(1)} M \supset \operatorname{Fil}^{(2)} M \supset \operatorname{Fil}^{(3)} M \supset \dots .$$

The completion $\widehat{M}$ of M with respect to this filtration is defined by the inverse limit

$$\widehat{M} = \varprojlim_{j} {M}/{\operatorname{Fil}^{(j)} M}.$$

If $\widehat{M} = M$, then M is called a complete R-module. The completion $\widehat{M}$ of M is also a filtered R-module via

$$\operatorname{Fil}^{(j)} \widehat{M} = \varprojlim_{k>j} {\operatorname{Fil}^{(j)} M}/{\operatorname{Fil}^{(k)} M}.$$

Proposition A.45. *Assume that* $M = \bigoplus_{i\geq 0} M^{(i)}$ *is a graded* R*-module. Then* M *admits a descending filtration given by* $\operatorname{Fil}^{(j)} M = \bigoplus_{i\geq j} M^{(i)}$. *Since* ${M}/{\operatorname{Fil}^{(j)} M} = \bigoplus_{i=0}^{j-1} M^{(i)}$, *the completion of* M *is*

$$\widehat{M} = \varprojlim_{j} {M}/{\operatorname{Fil}^{(j)} M} = \prod_{i\geq 0} M^{(i)}.$$

The completion $\widehat{M}$ *is filtered by* $\operatorname{Fil}^{(j)} \widehat{M} = \prod_{i\geq j} M^{(i)}$.

Proposition A.46. *Let* M, N *be two graded* R*-modules. Then the tensor product* $M \otimes N$ *is also graded (Lemma A.2) and for the completion* $M \hat{\otimes} N$ *one has*

$$M \hat{\otimes} N = \prod_{i\geq 0} \left(\bigoplus_{a+b=i} M^{(a)} \otimes N^{(b)} \right).$$

Moreover, there is a canonical embedding $M \otimes N \hookrightarrow M \hat{\otimes} N$. *We denote the image of* $m \otimes n \in M \otimes N$ *under this embedding by* $m \hat{\otimes} n$.

Definition A.47. Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a graded Hopf algebra (resp. bialgebra/ coalgebra/ algebra). By extending the maps $m, \eta, \Delta, \varepsilon, S$ of H to the completed module $\widehat{H}$, one obtains the completed Hopf algebra (resp. bialgebra/ coalgebra/ algebra) of H.

The completed Hopf algebra $(\widehat{H}, m, \eta, \Delta, \varepsilon, S)$ is filtered, i.e., one has for all $i \geq 0$

$$m(\operatorname{Fil}^{(i)} H \otimes \operatorname{Fil}^{(j)} H) \subset \operatorname{Fil}^{(i+j)} H, \qquad \Delta(\operatorname{Fil}^{(i)} H) \subset \sum_{m+n=i} \operatorname{Fil}^{(m)} H \otimes \operatorname{Fil}^{(n)} H,$$

$$S(\operatorname{Fil}^{(i)} H) \subset \operatorname{Fil}^{(i)} H.$$

Definition A.48. Let M be a filtered R-module. Then the associated graded module $\operatorname{gr} M$ is defined by

$$\operatorname{gr} M = \bigoplus_{j\geq 0} {\operatorname{Fil}^{(j)} M}/{\operatorname{Fil}^{(j+1)} M}.$$

One has $\operatorname{gr} M = \operatorname{gr} \widehat{M}$. In particular, if M is a graded module, then $\operatorname{gr} \widehat{M} = M$.

If M is a filtered R-module and all quotients ${M}/{\operatorname{Fil}^{(j)} M}$ are free modules of finite rank, then the module $\operatorname{gr} M$ is graded in the sense of Definition A.1.

Definition A.49. Let $(H, m, \eta, \Delta, \varepsilon, S)$ be a filtered Hopf algebra over R. Then the associated graded Hopf algebra is the R-module $\operatorname{gr} H$ equipped with the induced maps by $m, \eta, \Delta, \varepsilon$ and S.

Similarly, the associated graded for bialgebras, coalgebras, and algebras is defined.

Definition A.50. Let H be a graded Hopf algebra and denote by $\widehat{H} = \prod_{j\geq 0} H^{(j)}$ its completion. For an element $x \in \prod_{j\geq 1} H^{(j)} \subset \widehat{H}$, define

$$\exp_H(x) = \sum_{i\geq 0} \frac{1}{i!} x^i,$$

where x^i means applying the product map exactly $(i-1)$-times to $x^{\otimes i}$.

The map exp provides a bijection between the primitive and grouplike elements of a completed Hopf algebra.

Theorem A.51. *Let H be a graded Hopf algebra. Then there is a bijection*

$$\begin{aligned} \operatorname{Prim}(\widehat{H}) &\xrightarrow{\sim} \operatorname{Grp}(\widehat{H}), \\ x &\mapsto \exp_H(x). \end{aligned}$$

□

A.3 Quasi-shuffle algebras

This chapter provides an introduction to a special type of Hopf algebras, the quasi-shuffle Hopf algebras. All results are taken from the articles [Hof00] and [HI17]. In the following, R is some arbitrary fixed commutative $\mathbb{Q}$-algebra with unit.

Let $\mathcal{A}$ be an alphabet, this means $\mathcal{A}$ is a countable set whose elements are called letters. By $R\mathcal{A}$ denote the R-module spanned by the letters of $\mathcal{A}$ and let $R\langle\mathcal{A}\rangle$ be the free non-commutative algebra generated by the alphabet $\mathcal{A}$. The monic monomials in $R\langle\mathcal{A}\rangle$ are called words with letters in $\mathcal{A}$, the set of all words is denoted by $\mathcal{A}^*$. Moreover, let $\mathbf{1}$ be the empty word.

Definition A.52. Let $\diamond : R\mathcal{A} \times R\mathcal{A} \to R\mathcal{A}$ be a commutative and associative product. Define the quasi-shuffle product $*_\diamond$ on $R\langle\mathcal{A}\rangle$ recursively by $\mathbf{1} *_\diamond w = w *_\diamond \mathbf{1} = w$ and

$$au *_\diamond bv = a(u *_\diamond bv) + b(au *_\diamond v) + (a \diamond b)(u *_\diamond v)$$

for all $u, v, w \in R\langle\mathcal{A}\rangle$ and $a, b \in \mathcal{A}$.

Note that the quasi-shuffle product $*_\diamond$ can be equally defined recursively from the left and from the right, since both product expressions agree.

Example A.53. 1) Define $a \diamond b = 0$ for all $a, b \in \mathcal{A}$, then we get the well-known shuffle product, which is usually denoted by $\sqcup\!\sqcup$. Choosing the alphabet $\mathcal{X} = \{x_0, x_1\}$, the shuffle product occurs for multiple zeta values (Definition B.13).

2) Let $\mathcal{Y} = \{y_1, y_2, y_3, \ldots\}$ and define on $R\mathcal{Y}$ the product $y_i \diamond y_j = y_{i+j}$. The corresponding quasi-shuffle product is known as the stuffle product or harmonic product and is usually denoted by $*$, it arises in the context of multiple zeta values (Definition B.17).

3) Consider the alphabet $\mathcal{B} = \{b_0, b_1, b_2, \ldots\}$ and define on $R\mathcal{B}$ the product $b_i \diamond_{\mathrm{SZ}} b_j = b_{i+j}$. We will refer to this quasi-shuffle product as the SZ stuffle product, since it appears for the SZ multiple q-zeta values (Definition 2.11), and denote this by $*_{\mathrm{SZ}}$.

4) On the alphabet $\mathcal{B}$ define another product by

$$b_i \diamond_q b_j = \begin{cases} b_{i+j}, & \text{if } i, j \geq 1, \\ 0 & \text{else} \end{cases}.$$

This quasi-shuffle product occurs for balanced multiple q-zeta values (Definition 2.58) and will be called the balanced quasi-shuffle product, it is denoted by $*_q$.

5) Consider the bi-alphabet $\mathcal{Y}^{\mathrm{bi}} = \{y_{k,m} \mid k \geq 1,\ m \geq 0\}$. There are numbers $\lambda_j^{k_1,k_2} \in R$, such that one obtains an associative and commutative product

$$y_{k_1,m_1} \diamond y_{k_2,m_2} = y_{k_1+k_2,m_1+m_2} + \sum_{j=1}^{k_1+k_2-1} \lambda_j^{k_1,k_2} y_{j,m_1+m_2}. \tag{A.53.1}$$

In the context of bi-brackets (2.31.1), an explicit choice of the numbers $\lambda_j^{k_1,k_2}$ is given, and the corresponding quasi-shuffle product is denoted by $*_{\mathrm{bb}}$.

6) Another possible choice in A.53.1 is $\lambda_j^{k_1,k_2} = 0$ for all $j, k_1, k_2 \geq 1$, the obtained quasi-shuffle product is called the q-stuffle product and is denoted by $*$. This should be seen as a bi-version of the stuffle product on $R\langle\mathcal{Y}\rangle$ given in 2). It appears in the context of the combinatorial bi-multiple Eisenstein series (Definition 2.40).

Proposition A.54. *The pair* $(R\langle\mathcal{A}\rangle, *_\diamond)$ *is an associative, commutative algebra.* $\square$

For the shuffle algebra $(R\langle\mathcal{A}\rangle, ш)$ there is an explicit generating set. Choose a total ordering on the alphabet $\mathcal{A}$, then the lexicographic ordering defines a total ordering on the set of all words $\mathcal{A}^*$. Recall that a word $w \in \mathcal{A}^*\backslash\{\mathbf{1}\}$ is called a Lyndon word, if we have for any nontrivial decomposition $w = uv$ that $w < v$ (Definition A.12).

Theorem A.55. *([Re93, Theorem 4.9 (ii)]) The shuffle algebra* $(R\langle\mathcal{A}\rangle, ш)$ *is a free polynomial algebra generated by the Lyndon words of* $\mathcal{A}$. $\square$

We will see that all quasi-shuffle algebras over the same alphabet $\mathcal{A}$ are isomorphic. In particular, the previous theorem holds for all quasi-shuffle algebras.

Definition A.56. Let $(R\langle\mathcal{A}\rangle, *_\diamond)$ be a quasi-shuffle algebra. By a composition of a positive integer n we mean an ordered sequence $I = (i_1, \ldots, i_r)$, such that $i_1 + \cdots + i_r = n$. Let $w = a_1 \ldots a_n \in \mathcal{A}^*$ be a word and $I = (i_1, \ldots, i_r)$ a composition of n, then define

$$I[w] = (a_1 \diamond \cdots \diamond a_{i_1})(a_{i_1+1} \diamond \cdots \diamond a_{i_1+i_2}) \ldots (a_{i_1+\cdots+i_{r-1}+1} \diamond \cdots \diamond a_n)$$

and

$$\begin{aligned}
\exp_{*_\diamond}(w) &= \sum_{I=(i_1,\ldots,i_r) \text{ composition of } n} \frac{1}{i_1! \ldots i_r!} I[w], \\
\log_{*_\diamond}(w) &= \sum_{I=(i_1,\ldots,i_r) \text{ composition of } n} \frac{(-1)^{n-r}}{i_1 \ldots i_r} I[w].
\end{aligned}$$

Theorem A.57. *([Hof00, Theorem 2.5]) The map* $\exp_{*_\diamond}$ *is an algebra isomorphism*

$$\exp_{*_\diamond} : (R\langle\mathcal{A}\rangle, ш) \xrightarrow{\sim} (R\langle\mathcal{A}\rangle, *_\diamond).$$

The inverse map is given by $\log_{*_\diamond}$. $\square$

From Theorem A.55 and A.57, one deduces the following.

Corollary A.58. *Any quasi-shuffle algebra* $(R\langle\mathcal{A}\rangle, *_\diamond)$ *is a free polynomial algebra generated by the Lyndon words of* $\mathcal{A}$.

Next, we equip the quasi-shuffle algebras with a Hopf algebra structure. Define the deconcatenation coproduct $\Delta_{\text{dec}} : R\langle\mathcal{A}\rangle \to R\langle\mathcal{A}\rangle \otimes R\langle\mathcal{A}\rangle$ and the counit map $\varepsilon : R\langle\mathcal{A}\rangle \to R$ for a word $w \in \mathcal{A}^*$ by

$$\Delta_{\text{dec}}(w) = \sum_{w=uv} u \otimes v, \qquad \varepsilon(w) = \begin{cases} 1, & \text{if } w = \mathbf{1} \\ 0 & \text{else} \end{cases}. \tag{A.58.1}$$

Theorem A.59. *([Hof00, Theorem 3.1, 3.2]) The tuple* $(R\langle\mathcal{A}\rangle, *_\diamond, \mathbf{1}, \Delta_{\text{dec}}, \varepsilon)$ *is a commutative Hopf algebra.* $\square$

The antipode $S_{*_\diamond} : R\langle\mathcal{A}\rangle \to R\langle\mathcal{A}\rangle$ is on a word $w = a_1 \ldots a_n$ in $\mathcal{A}^*$ given by

$$S_{*_\diamond}(w) = (-1)^n \sum_{I=(i_1,\ldots,i_r) \text{ composition of } n} I[a_n a_{n-1} \ldots a_1].$$

The map $\exp_{*_\diamond}$ in Theorem A.57 is compatible with the Hopf algebra structures, explicitly the following holds.

Theorem A.60. *([Hof00, Theorem 3.3]) The map* $\exp_{*_\diamond}$ *is a Hopf algebra isomorphism*

$$\exp_{*_\diamond} : (R\langle\mathcal{A}\rangle, ш, \mathbf{1}, \Delta_{\text{dec}}, \varepsilon) \xrightarrow{\sim} (R\langle\mathcal{A}\rangle, *_\diamond, \mathbf{1}, \Delta_{\text{dec}}, \varepsilon).$$

□

We want to determine a completed dual of the quasi-shuffle Hopf algebra (in the sense of Definition A.18). Define a degree map on the letters in $\mathcal{A}$, such that $\deg(a) \geq 1$ for all $a \in \mathcal{A}$. This induces a grading on the quasi-shuffle Hopf algebra $(R\langle\mathcal{A}\rangle, *_\diamond, \mathbf{1}, \Delta_{\text{dec}}, \varepsilon)$ by

$$\deg(a_1 \dots a_n) = \deg(a_1) + \dots + \deg(a_n), \qquad a_1, \dots, a_n \in \mathcal{A}.$$

Denote by $R\langle\langle\mathcal{A}\rangle\rangle$ the completion with respect to this grading (see Proposition A.45). There is a pairing

$$\begin{aligned} (\cdot \mid \cdot) : R\langle\langle\mathcal{A}\rangle\rangle \otimes R\langle\mathcal{A}\rangle &\to R, \\ \phi \otimes w &\mapsto (\phi \mid w), \end{aligned} \tag{A.60.1}$$

where $(\phi \mid w)$ denotes the coefficient of $\phi \in R\langle\langle\mathcal{A}\rangle\rangle$ in $w \in R\langle\mathcal{A}\rangle$. On $R\langle\langle\mathcal{A}\rangle\rangle$ define the coproduct $\Delta_{*_\diamond} : R\langle\langle\mathcal{A}\rangle\rangle \to R\langle\langle\mathcal{A}\rangle\rangle \otimes R\langle\langle\mathcal{A}\rangle\rangle$ by

$$\Delta_{*_\diamond}(\phi) = \sum_{u,v \in \mathcal{A}^*} (\phi \mid u *_\diamond v)\ u \otimes v.$$

Moreover, denote the concatenation product by conc.

Theorem A.61. *The tuple* $(R\langle\langle\mathcal{A}\rangle\rangle, \text{conc}, \mathbf{1}, \Delta_{*_\diamond}, \varepsilon)$ *is a complete cocommutative Hopf algebra. It is dual to the quasi-shuffle Hopf algebra* $(R\langle\mathcal{A}\rangle, *_\diamond, \mathbf{1}, \Delta_{\text{dec}}, \varepsilon)$ *with respect to the pairing* $(\cdot \mid \cdot)$ *given in* (A.60.1). □

Example A.62. For the shuffle product ш given in Example A.53 1), the dual coproduct is given by

$$\Delta_ш(a) = a \otimes \mathbf{1} + \mathbf{1} \otimes a \qquad \text{for all } a \in \mathcal{A}.$$

So $(R\langle\langle\mathcal{A}\rangle\rangle, \text{conc}, \Delta_ш)$ is a cocommutative Hopf algebra (cf. Corollary A.40).

Let $\exp^\vee_{*_\diamond}$ the algebra endomorphism on $(R\langle\langle\mathcal{A}\rangle\rangle, \text{conc})$ defined by

$$\exp^\vee_{*_\diamond}(a) = \sum_{a_1 \diamond \dots \diamond a_n = a} \frac{1}{n!} a_1 \dots a_n$$

for all letters $a \in \mathcal{A}$. Then by duality, the following holds

Corollary A.63. *([Hof00, Theorem 4.1]) The map* $\exp^\vee_{*_\diamond}$ *gives a Hopf algebra isomorphism*

$$\exp^\vee_{*_\diamond} : (R\langle\langle\mathcal{A}\rangle\rangle, \text{conc}, \mathbf{1}, \Delta_{*_\diamond}, \varepsilon) \to (R\langle\langle\mathcal{A}\rangle\rangle, \text{conc}, \mathbf{1}, \Delta_ш, \varepsilon).$$

□

A.4 Generating series and quasi-shuffle products

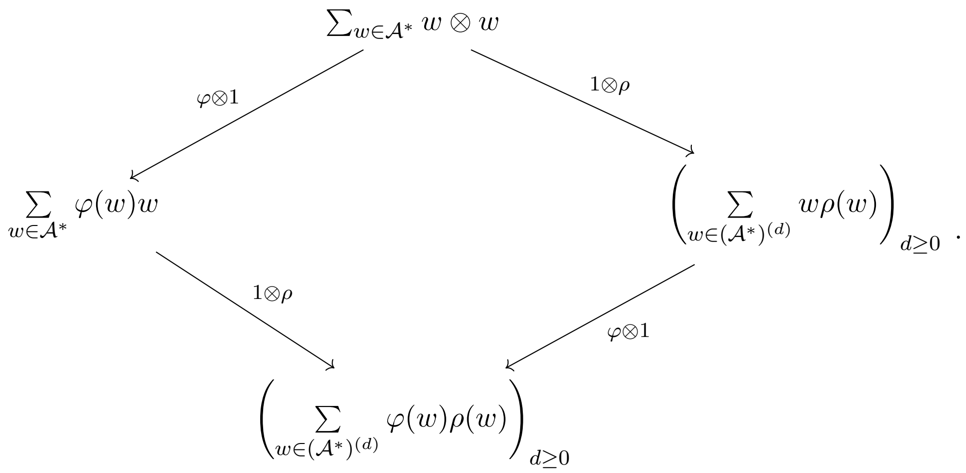
For a quasi-shuffle algebra $(\mathbb{Q}\langle\mathcal{A}\rangle, *_\diamond)$ we want to study its symmetries in terms of generating series. In all our given examples the quasi-shuffle algebra $(\mathbb{Q}\langle\mathcal{A}\rangle, *_\diamond)$ will be filtered or graded. Define the generic diagonal series of $\mathbb{Q}\langle\mathcal{A}\rangle$ by

$$\mathcal{W}(\mathcal{A}) = \sum_{w\in\mathcal{A}^*} w \otimes w.$$

We want to apply $\mathbb{Q}$-linear maps to the first factors, usually denoted by φ, or to the second factors, usually denoted by ρ, of $\mathcal{W}(\mathcal{A})$ to get generating series of different kinds and describe the resulting properties.
Let $\mathrm{dep} : \mathcal{A}^* \to \mathbb{Z}_{\geq 0}$ be a depth map compatible with concatenation, i.e., we have

$$\mathrm{dep}(uv) = \mathrm{dep}(u) + \mathrm{dep}(v), \qquad u, v \in \mathcal{A}^*.$$

Denote by $(\mathcal{A}^*)^{(d)}$ the set of all words in $\mathcal{A}^*$ of depth d and by $\mathbb{Q}\langle\mathcal{A}\rangle^{(d)}$ the space spanned by $(\mathcal{A}^*)^{(d)}$. Then in the following, we will explain the following picture



We begin with an abstract discussion and later a more detailed explanation in special cases is given.

Definition A.64. Let $\rho_\mathcal{A} : \mathbb{Q}\langle\mathcal{A}\rangle \to \mathbb{Q}[Z_1, Z_2, \ldots]$ be a $\mathbb{Q}$-linear map having the following properties with respect to the depth map

(i) For each $d \geq 1$, the restriction of $\rho_\mathcal{A}$ to $\mathbb{Q}\langle\mathcal{A}\rangle^{(d)}$ is an injective $\mathbb{Q}$-linear map

$$\rho_\mathcal{A}|_{\mathbb{Q}\langle\mathcal{A}\rangle^{(d)}} : \mathbb{Q}\langle\mathcal{A}\rangle^{(d)} \to \mathbb{Q}[Z_1, \ldots, Z_d].$$

(ii) For $n \geq 1$ denote by $\rho_\mathcal{A}^{[n]}$ the $\mathbb{Q}$-linear map obtained from $\rho_\mathcal{A}$ by shifting the variables Z_i to Z_{n+i}, so $\rho_\mathcal{A}^{[n]}\left(\mathbb{Q}\langle\mathcal{A}\rangle^{(d)}\right) \subset \mathbb{Q}[Z_{n+1}, \ldots, Z_{n+d}]$. Then, one has

$$\rho_\mathcal{A}(uv) = \rho_\mathcal{A}(u)\rho_\mathcal{A}^{[n]}(v), \qquad u \in \mathbb{Q}\langle\mathcal{A}\rangle^{(n)},\ v \in \mathbb{Q}\langle\mathcal{A}\rangle.$$

Definition A.65. Let $\rho_\mathcal{A} : \mathbb{Q}\langle\mathcal{A}\rangle \to \mathbb{Q}[Z_1, Z_2, \ldots]$ be a $\mathbb{Q}$-linear map as in Definition A.64. The (commutative) generating series of words in $\mathbb{Q}\langle\mathcal{A}\rangle$ associated to $\rho_\mathcal{A}$ are given by $\rho_\mathcal{A}(\mathcal{W})_0 = \mathbf{1}$ and for $d \geq 1$ by

$$\rho_\mathcal{A}(\mathcal{W})_d(Z_1, \ldots, Z_d) = \sum_{w\in(\mathcal{A}^*)^{(d)}} w\rho(w) \in \mathbb{Q}\langle\mathcal{A}\rangle[[Z_1, \ldots, Z_d]].$$

For simplicity, we will usually omit the index d and just write $\rho_{\mathcal{A}}(\mathcal{W})(Z_1,\ldots,Z_d)$ for the generating series of words in depth d.

Extend the concatenation product defined on $\mathbb{Q}\langle\mathcal{A}\rangle$ to $\mathbb{Q}\langle\mathcal{A}\rangle[[Z_1,Z_2,\ldots]]$ by $\mathbb{Q}[[Z_1,Z_2,\ldots]]$-linearity and denote it by $\cdot$. Then there is an explicit expression of the concatenation product on the generating series of words $\rho_{\mathcal{A}}(\mathcal{W})$.

Proposition A.66. *Let $\rho_{\mathcal{A}}:\mathbb{Q}\langle A\rangle\to\mathbb{Q}[Z_1,Z_2,\ldots]$ be a $\mathbb{Q}$-linear map as in Definition A.64. Then for $0\le n\le d$, one has*

$$\rho_{\mathcal{A}}(\mathcal{W})(Z_1,\ldots,Z_n)\cdot\rho_{\mathcal{A}}(\mathcal{W})(Z_{n+1},\ldots,Z_d)=\rho_{\mathcal{A}}(\mathcal{W})(Z_1,\ldots,Z_d).$$

Proof. For $n=0,d$ the formula is obvious. For $0<n<d$, compute

$$\begin{aligned}\rho_{\mathcal{A}}(\mathcal{W})(Z_1,\ldots,Z_n)\cdot\rho_{\mathcal{A}}(\mathcal{W})(Z_{n+1},\ldots,Z_d)&=\sum_{u\in(\mathcal{A}^*)^{(n)}}\sum_{v\in(\mathcal{A}^*)^{(d-n)}}uv\rho_{\mathcal{A}}(u)\rho_{\mathcal{A}}^{[n]}(v)\\ =\sum_{u\in(\mathcal{A}^*)^{(n)}}\sum_{v\in(\mathcal{A}^*)^{(d-n)}}uv\rho_{\mathcal{A}}(uv)&=\sum_{w\in(\mathcal{A}^*)^{(d)}}w\rho_{\mathcal{A}}(w)=\rho_{\mathcal{A}}(\mathcal{W})(Z_1,\ldots,Z_d).\end{aligned}$$

□

Extend also the quasi-shuffle product $*_\diamond$ on $\mathbb{Q}\langle\mathcal{A}\rangle$ to $\mathbb{Q}\langle\mathcal{A}\rangle[[Z_1,Z_2,\ldots]]$ by $\mathbb{Q}[[Z_1,Z_2,\ldots]]$-linearity. Then by definition of the quasi-shuffle product $*_\diamond$, we have that for all $0\le n\le d$

$$\rho_{\mathcal{A}}(\mathcal{W})(Z_1,\ldots,Z_n)*_\diamond\rho_{\mathcal{A}}(\mathcal{W})(Z_{n+1},\ldots,Z_d)\in\mathbb{Q}\langle\mathcal{A}\rangle[[Z_1,\ldots,Z_d]].$$

In some special cases, this expression can be described explicitly by a recursive formula.

Consider the alphabet $\mathcal{Y}=\{y_1,y_2,\ldots\}$. For a word in $\mathbb{Q}\langle\mathcal{Y}\rangle$ define the depth as

$$\operatorname{dep}(y_{k_1}\ldots y_{k_d})=d,\qquad k_1,\ldots,k_d\ge 1,$$

and let $\rho_{\mathcal{Y}}$ be the $\mathbb{Q}$-linear map defined by

$$\begin{aligned}\rho_{\mathcal{Y}}:\mathbb{Q}\langle\mathcal{Y}\rangle&\to\mathbb{Q}[X_1,X_2,\ldots],\\ y_{k_1}\ldots y_{k_d}&\mapsto X_1^{k_1-1}\ldots X_d^{k_d-1}.\end{aligned}\tag{A.66.1}$$

It is obvious that the map $\rho_{\mathcal{Y}}$ satisfies the properties listed in Definition A.64 and the associated generating series of words are given by $\rho_{\mathcal{Y}}(\mathcal{W})_0=\mathbf{1}$ and

$$\rho_{\mathcal{Y}}(\mathcal{W})_d(X_1,\ldots,X_d)=\sum_{k_1,\ldots,k_d\ge1}y_{k_1}\ldots y_{k_d}X_1^{k_1-1}\ldots X_d^{k_d-1},\quad d\ge1.$$

Proposition A.67. *(i) Let $(\mathbb{Q}\langle\mathcal{Y}\rangle,ш)$ be the shuffle algebra, i.e., ш is the quasi-shuffle product corresponding to $y_i\diamond y_j=0$ for all $i,j\ge1$ (Example A.53 1)). Then we have for all $0<n<d$ that $\mathbf{1}ш\rho_{\mathcal{Y}}(\mathcal{W})_n=\rho_{\mathcal{Y}}(\mathcal{W})_nш\mathbf{1}=\rho_{\mathcal{Y}}(\mathcal{W})_n$ and*

$$\begin{aligned}&\rho_{\mathcal{Y}}(\mathcal{W})(X_1,\ldots,X_n)ш\rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1},\ldots,X_d)\\&\qquad=\rho_{\mathcal{Y}}(\mathcal{W})(X_1)\cdot\Big(\rho_{\mathcal{Y}}(\mathcal{W})(X_2,\ldots,X_n)ш\rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1},\ldots,X_d)\Big)\\&\qquad+\rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1})\cdot\Big(\rho_{\mathcal{Y}}(\mathcal{W})(X_1,\ldots,X_n)ш\rho_{\mathcal{Y}}(\mathcal{W})(X_{n+2},\ldots,X_d)\Big).\end{aligned}$$

(ii) ([Ih07, Proposition 8 (i)]) Let $(\mathbb{Q}\langle\mathcal{Y}\rangle,*)$ be the stuffle algebra, i.e., $*$ is the quasi-shuffle product with $y_i\diamond y_j=y_{i+j}$ for all $i,j\ge1$ (Example A.53 2)). One obtains for all

$0 < n < d$ *that* $\mathbf{1} * \rho_{\mathcal{Y}}(\mathcal{W})_n = \rho_{\mathcal{Y}}(\mathcal{W})_n * \mathbf{1} = \rho_{\mathcal{Y}}(\mathcal{W})_n$ *and*

$$\begin{aligned}\rho_{\mathcal{Y}}(\mathcal{W})(X_1,\dots,X_n) * \rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1},\dots,X_d)\\ &= \rho_{\mathcal{Y}}(\mathcal{W})(X_1)\cdot\Big(\rho_{\mathcal{Y}}(\mathcal{W})(X_2,\dots,X_n) * \rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1},\dots,X_d)\Big)\\ &+ \rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1})\cdot\Big(\rho_{\mathcal{Y}}(\mathcal{W})(X_1,\dots,X_n) * \rho_{\mathcal{Y}}(\mathcal{W})(X_{n+2},\dots,X_d)\Big)\\ &+ \frac{\rho_{\mathcal{Y}}(\mathcal{W})(X_1)-\rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1})}{X_1-X_{n+1}}\cdot\Big(\rho_{\mathcal{Y}}(\mathcal{W})(X_2,\dots,X_n) * \rho_{\mathcal{Y}}(\mathcal{W})(X_{n+2},\dots,X_d)\Big).\end{aligned}$$

Proof. We only prove (ii). Part (i) follows then from (ii) by applying the same calculations and arguments modulo lower depth. First, restrict to the case $d = 2$ and compute directly

$$\begin{aligned}\rho_{\mathcal{Y}}(\mathcal{W})(X_1) *_q \rho_{\mathcal{Y}}(\mathcal{W})(X_2)\\ &= \sum_{k_1,k_2\geq 1}(y_{k_1} * y_{k_2})X_1^{k_1-1}X_2^{k_2-1} = \sum_{k_1,k_2\geq 1}\Big(y_{k_1}y_{k_2}+y_{k_2}y_{k_1}+y_{k_1+k_2}\Big)X_1^{k_1-1}X_2^{k_2-1}\\ &= \rho_{\mathcal{Y}}(\mathcal{W})(X_1,X_2)+\rho_{\mathcal{Y}}(\mathcal{W})(X_2,X_1)+\frac{\rho_{\mathcal{Y}}(\mathcal{W})(X_1)-\rho_{\mathcal{Y}}(\mathcal{W})(X_2)}{X_1-X_2},\end{aligned}$$

where

$$\sum_{k_1,k_2\geq 1} y_{k_1+k_2}X_1^{k_1-1}X_2^{k_2-1} = \frac{\rho_{\mathcal{Y}}(\mathcal{W})(X_1)-\rho_{\mathcal{Y}}(\mathcal{W})(X_2)}{X_1-X_2}$$

follows from a simple power series manipulation. Since the stuffle product as well as the above generating series formula are given recursively, we obtain the claim in arbitrary depth by applying induction and the same arguments as before. □

Next, consider the alphabet $\mathcal{X} = \{x_0, x_1\}$ and let $\mathfrak{h}^1$ be the subalgebra of $\mathbb{Q}\langle\mathcal{X}\rangle$ spanned by all words ending in x_1. For a word in $\mathfrak{h}^1$ define the depth as

$$\operatorname{dep}(x_0^{k_1-1}x_1\dots x_0^{k_d-1}x_1) = d, \qquad k_1,\dots,k_d \geq 1,$$

and let $\rho_{\mathcal{X}}$ be the $\mathbb{Q}$-linear map defined by

$$\begin{aligned}\rho_{\mathcal{X}} : \mathfrak{h}^1 &\to \mathbb{Q}[X_1,X_2,\dots],\\ x_0^{k_1-1}x_1\dots x_0^{k_d-1}x_1 &\mapsto X_1^{k_1-1}\dots X_d^{k_d-1}.\end{aligned}$$

The map $\rho_{\mathcal{X}}$ satisfies the properties in Definition A.64 and the generating series of words associated to $\rho_{\mathcal{X}}$ is given by $\rho_{\mathcal{X}}(\mathcal{W})_0 = \mathbf{1}$ and

$$\rho_{\mathcal{X}}(\mathcal{W})_d(X_1,\dots,X_d) = \sum_{k_1,\dots,k_d\geq 1} x_0^{k_1-1}x_1\dots x_d^{k_d-1}x_1X_1^{k_1-1}\dots X_d^{k_d-1}, \quad d\geq 1.$$

Proposition A.68. *([Ih07, Proposition 8 (ii)]) Let* $(\mathfrak{h}^1, ш)$ *be the shuffle algebra, i.e.,* ш *is the quasi-shuffle product with* $x_i \diamond x_j = 0$ *for* $i,j\in\{0,1\}$ *(Example A.53 1)). We obtain for* $0 < n < d$ *that* $\mathbf{1} ш \rho_{\mathcal{X}}(\mathcal{W})_n = \rho_{\mathcal{X}}(\mathcal{W})_n ш \mathbf{1} = \rho_{\mathcal{X}}(\mathcal{W})_n$ *and*

$$\begin{aligned}\rho_{\mathcal{X}}(\mathcal{W})(X_1,\dots,X_n) ш \rho_{\mathcal{X}}(\mathcal{W})(X_{n+1},\dots,X_d)\\ &= \rho_{\mathcal{X}}(\mathcal{W})(X_1+X_{n+1})\cdot\Big(\rho_{\mathcal{X}}(\mathcal{W})(X_2,\dots,X_n) ш \rho_{\mathcal{X}}(\mathcal{W})(X_{n+1},\dots,X_d)\Big)\\ &+ \rho_{\mathcal{X}}(\mathcal{W})(X_1+X_{n+1})\cdot\Big(\rho_{\mathcal{X}}(\mathcal{W})(X_1,\dots,X_n) ш \rho_{\mathcal{X}}(\mathcal{W})(X_{n+2},\dots,X_d)\Big).\end{aligned}$$

Proof. First, restrict to the case $d = 2$ and obtain

$$\rho_{\mathcal{X}}(\mathcal{W})(X_1) = \frac{\mathbf{1}}{\mathbf{1} - x_0 X_1} \cdot x_1, \tag{A.68.1}$$

$$= x_1 + x_0 X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1). \tag{A.68.2}$$

Thus, compute

$$\begin{aligned}
&\rho_{\mathcal{X}}(\mathcal{W})(X_1) \sqcup\!\sqcup \rho_{\mathcal{X}}(\mathcal{W})(X_2) \\
&= x_1 \sqcup\!\sqcup x_1 + x_1 \sqcup\!\sqcup \Big(x_0 X_2 \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big) + \Big(x_0 X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1)\Big) \sqcup\!\sqcup x_1 \\
&\quad + \Big(x_0 X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1)\Big) \sqcup\!\sqcup \Big(x_0 X_2 \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big) \\
&= 2x_1^2 + x_1 \cdot x_0 X_2 \rho_{\mathcal{X}}(\mathcal{W})(X_2) + x_0 \cdot \Big(x_1 \sqcup\!\sqcup \Big(X_2 \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big)\Big) + x_1 \cdot x_0 X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1) \\
&\quad + x_0 \cdot \Big(\Big(X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1) \sqcup\!\sqcup x_1\Big)\Big) + x_0 \cdot \Big(\Big(X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1)\Big) \sqcup\!\sqcup \Big(x_0 X_2 \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big)\Big) \\
&\quad + x_0 \cdot \Big(\Big(x_0 X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1)\Big) \sqcup\!\sqcup X_2 \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big) \\
&= 2x_1^2 + x_1 \cdot \Big(\rho_{\mathcal{X}}(\mathcal{W})(X_2) - x_1\Big) + x_0 \cdot \Big(x_1 \sqcup\!\sqcup \Big(X_2 \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big)\Big) \\
&\quad + x_1 \cdot \Big(\rho_{\mathcal{X}}(\mathcal{W})(X_1) - x_1\Big) + x_0 \cdot \Big(\Big(X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1) \sqcup\!\sqcup x_1\Big)\Big) \\
&\quad + x_0 \cdot \Big(\Big(X_1 \rho_{\mathcal{X}}(\mathcal{W})(X_1)\Big) \sqcup\!\sqcup \Big(\rho_{\mathcal{X}}(\mathcal{W})(X_2) - x_1\Big)\Big) \\
&\quad + x_0 \cdot \Big(\Big(\rho_{\mathcal{X}}(\mathcal{W})(X_1) - x_1\Big) \sqcup\!\sqcup X_2 \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big) \\
&= x_1 \cdot \rho_{\mathcal{X}}(\mathcal{W})(X_2) + x_1 \cdot \rho_{\mathcal{X}}(\mathcal{W})(X_1) + x_0(X_1 + X_2) \cdot \Big(\rho_{\mathcal{X}}(\mathcal{W})(X_1) \sqcup\!\sqcup \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big),
\end{aligned}$$

where the first equality follows from (A.68.2), the second equality is just applying the definition of $\sqcup\!\sqcup$, the third equality is again obtained from (A.68.2) and the fourth equality is simple cancellation and reordering. Together with (A.68.1) and Proposition A.66, one deduces

$$\begin{aligned}
\rho_{\mathcal{X}}(\mathcal{W})(X_1) \sqcup\!\sqcup \rho_{\mathcal{X}}(\mathcal{W})(X_2) &= \frac{\mathbf{1}}{\mathbf{1} - x_0(X_1 + X_2)} \cdot \Big(x_1 \cdot \rho_{\mathcal{X}}(\mathcal{W})(X_1) + x_1 \cdot \rho_{\mathcal{X}}(\mathcal{W})(X_2)\Big) \\
&= \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2) \cdot \rho_{\mathcal{X}}(\mathcal{W})(X_1) + \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2) \cdot \rho_{\mathcal{X}}(\mathcal{W})(X_2) \\
&= \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2, X_1) + \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2, X_2).
\end{aligned}$$

This is exactly the claimed formula for the generating series in depth 2. Since both the shuffle product and the generating series formula are defined recursively, the claim in arbitrary depths follows from induction. □

Remark A.69. Consider the isomorphism of vector spaces

$$\iota_{\mathcal{Y},\mathcal{X}} : \mathbb{Q}\langle\mathcal{Y}\rangle \to \mathfrak{h}^1, \quad y_{k_1} \dots y_{k_d} \mapsto x_0^{k_1-1} x_1 \dots x_0^{k_d-1} x_1$$

and extend it to $\mathbb{Q}\langle\mathcal{Y}\rangle[[X_1, X_2, \dots]]$ by $\mathbb{Q}[[X_1, X_2, \dots]]$-linearity. As obtained in [IKZ06] one has for all $0 < n < d$ that

$$\begin{aligned}
&(\rho_{\mathcal{X}}(\mathcal{W}))^{\#_{\mathcal{X}}}(X_1, \dots, X_n) \sqcup\!\sqcup (\rho_{\mathcal{X}}(\mathcal{W}))^{\#_{\mathcal{X}}}(X_{n+1}, \dots, X_d) \qquad \text{(A.69.1)} \\
&\qquad = \iota_{\mathcal{Y},\mathcal{X}} \left(\rho_{\mathcal{Y}}(\mathcal{W})(X_1, \dots, X_n) \sqcup\!\sqcup \rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1}, \dots, X_d)\right)^{\#_{\mathcal{X}}}.
\end{aligned}$$

Here the right-hand side is explained in Proposition A.67 (i) and we denote

$$(\rho_{\mathcal{X}}(\mathcal{W}))^{\#_{\mathcal{X}}}(X_1, \dots, X_d) = \rho_{\mathcal{X}}(\mathcal{W})(X_1 + \dots + X_d, X_2 + \dots + X_d, \dots, X_d).$$

By variable substitution, one shows that the formulas in (A.69.1) and in Proposition A.68 agree. For example, for $n = 1,\ d = 3$ the formula (A.69.1) reads

$$\begin{aligned}
&\rho_{\mathcal{X}}(\mathcal{W})(X_1) \sqcup\!\sqcup\, \rho_{\mathcal{X}}(\mathcal{W})(X_2 + X_3, X_3) \\
&\qquad = \iota_{\mathcal{Y},\mathcal{X}}\left(\rho_{\mathcal{Y}}(\mathcal{W})(X_1, X_2, X_3) + \rho_{\mathcal{Y}}(\mathcal{W})(X_2, X_1, X_3) + \rho_{\mathcal{Y}}(\mathcal{W})(X_2, X_3, X_1)\right)^{\#_{\mathcal{X}}} \\
&\qquad = \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2 + X_3, X_2 + X_3, X_3) + \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2 + X_3, X_1 + X_3, X_3) \\
&\qquad\quad + \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2 + X_3, X_1 + X_3, X_1).
\end{aligned}$$

Substituting $X_1 \mapsto X_1,\ X_2 \mapsto X_2 - X_3,\ X_3 \mapsto X_3$ this equation is equivalent to

$$\begin{aligned}
\rho_{\mathcal{X}}(\mathcal{W})(X_1) \sqcup\!\sqcup\, \rho_{\mathcal{X}}(\mathcal{W})(X_2, X_3) &= \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2, X_2, X_3) \\
&\quad + \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2, X_1 + X_3, X_3) + \rho_{\mathcal{X}}(\mathcal{W})(X_1 + X_2, X_1 + X_3, X_1),
\end{aligned}$$

which is exactly the formula in Proposition A.68 for $n = 1,\ d = 3$.

As a second step, we apply a $\mathbb{Q}$-linear map $\varphi : \mathbb{Q}\langle\mathcal{A}\rangle \to R$ into some commutative $\mathbb{Q}$-algebra R with unit to the first component of such a generating series of words $\rho_{\mathcal{A}}(\mathcal{W})$. In other words, we consider the image of the generic diagonal series $\mathcal{W}(\mathcal{A})$ under $\varphi \otimes \rho_{\mathcal{A}}$.

Definition A.70. Let $\rho_{\mathcal{A}} : \mathbb{Q}\langle\mathcal{A}\rangle \to \mathbb{Q}[Z_1, Z_2, \ldots]$ be a $\mathbb{Q}$-linear map as in Definition A.64, R be a commutative $\mathbb{Q}$-algebra with unit and $\varphi : \mathbb{Q}\langle\mathcal{A}\rangle \to R$ a $\mathbb{Q}$-linear map. Then the generating series with coefficients in R associated to $(\varphi, \rho_{\mathcal{A}})$ are given by $(\varphi\otimes\rho_{\mathcal{A}})(\mathcal{W})_0 = 1$ and

$$(\varphi \otimes \rho_{\mathcal{A}})(\mathcal{W})_d(Z_1, \ldots, Z_d) = \sum_{w \in (\mathcal{A}^*)^{(d)}} \varphi(w)\rho_{\mathcal{A}}(w) \in R[[Z_1, \ldots, Z_d]], \quad d \geq 1.$$

As before, we will usually drop the depth index and simply write $(\varphi\otimes\rho_{\mathcal{A}})(\mathcal{W})(Z_1, \ldots, Z_d)$. Later, we will refer to the sequences $(\varphi \otimes \rho_{\mathcal{A}})(\mathcal{W}) = \Big((\varphi \otimes \rho_{\mathcal{A}})(\mathcal{W})_d\Big)_{d\geq 0}$ as moulds or bimoulds (cf Section C).

Definition A.70 allows relating a quasi-shuffle product defined on $\mathbb{Q}\langle\mathcal{A}\rangle$ to a symmetry among a sequence in $\prod_{d\geq 0} R[[Z_1, \ldots, Z_d]]$.

Definition A.71. Let R be a commutative $\mathbb{Q}$-algebra with unit. A sequence $M = (M_d)_{d\geq 0} \in \prod_{d\geq 0} R[[Z_1, \ldots, Z_d]]$ is called $(\varphi_{*_\diamond}, \rho_{\mathcal{A}})$-symmetric if there is a $\mathbb{Q}$-algebra morphism $\varphi_{*_\diamond} : (\mathbb{Q}\langle\mathcal{A}\rangle, *_\diamond) \to (R, \cdot)$ and a $\mathbb{Q}$-linear map $\rho_{\mathcal{A}} : \mathbb{Q}\langle\mathcal{A}\rangle \to \mathbb{Q}[[Z_1, Z_2, \ldots]]$ satisfying the conditions in Definition A.64, such that for all $d \geq 0$

$$M_d = (\varphi_{*_\diamond} \otimes \rho_{\mathcal{A}})(\mathcal{W})_d.$$

Let $M = (M_d)_{d\geq 0} \in \prod_{d\geq 0} R[[Z_1, \ldots, Z_d]]$ be such a $(\varphi_{*_\diamond}, \rho_{\mathcal{A}})$-symmetric sequence. Then, one obtains immediately from the definition that for $0 < n < d$

$$\begin{aligned}
&M_n(Z_1, \ldots, Z_n)M_{d-n}(Z_{n+1}, \ldots, Z_d) && \text{(A.71.1)} \\
&\qquad = \varphi_{*_\diamond}\Big(\rho_{\mathcal{A}}(\mathcal{W})_n(Z_1, \ldots, Z_n) *_\diamond \rho_{\mathcal{A}}(\mathcal{W})_{d-n}(Z_{n+1}, \ldots, Z_d)\Big).
\end{aligned}$$

The right-hand side is an element in $\mathbb{Q}\langle\mathcal{A}\rangle[[Z_1, \ldots, Z_d]]$, so we need to extend the map $\varphi_{*_\diamond} : \mathbb{Q}\langle\mathcal{A}\rangle \to R$ by $\mathbb{Q}[[Z_1, Z_2, \ldots]]$-linearity to apply it to this expression.

Example A.72. Recall that the map

$$\begin{aligned}\rho_{\mathcal{Y}} : \mathbb{Q}\langle\mathcal{Y}\rangle &\to \mathbb{Q}[X_1, X_2, \ldots],\\ y_{k_1}\ldots y_{k_d} &\mapsto X_1^{k_1-1}\ldots X_d^{k_d-1}.\end{aligned}$$

given in (A.66.1) satisfies the conditions in Definition A.64.

1) A sequence $M = (M_d)_{d\geq 0} \in R[[X_1, \ldots, X_d]]$ will be called symmetral if there is an algebra morphism $\varphi_{⧢} : (\mathbb{Q}\langle\mathcal{Y}\rangle, ⧢) \to R$, such that M is $(\varphi_{⧢}, \rho_{\mathcal{Y}})$-symmetric. So M is symmetral if and only if we have for all $0 < n < d$

$$M_n(X_1, \ldots, X_n)M_{d-n}(X_{n+1}, \ldots, X_d) \\ = \varphi_{⧢}\Big(\rho_{\mathcal{Y}}(\mathcal{W})_n(X_1, \ldots, X_n) ⧢ \rho_{\mathcal{Y}}(\mathcal{W})_{d-n}(X_{n+1}, \ldots, X_d)\Big),$$

where the right-hand side is explicitly described in Proposition A.67 (i).

2) A sequence $M = (M_d)_{d\geq 0} \in R[[X_1, \ldots, X_d]]$ will be called symmetril if there is an algebra morphism $\varphi_* : (\mathbb{Q}\langle\mathcal{Y}\rangle, *) \to R$, such that M is $(\varphi_*, \rho_{\mathcal{Y}})$-symmetric. In particular, M is symmetril if and only if we have for all $0 < n < d$

$$M_n(X_1, \ldots, X_n)M_{d-n}(X_{n+1}, \ldots, X_d) \\ = \varphi_*\Big(\rho_{\mathcal{Y}}(\mathcal{W})_n(X_1, \ldots, X_n) * \rho_{\mathcal{Y}}(\mathcal{W})_{d-n}(X_{n+1}, \ldots, X_d)\Big).$$

An explicit expression for the right hand-side is given in Proposition A.67 (ii).

Definition A.71 will be used in Subsection 2.7 and C.1 to obtain the definition of symmetral, symmetril, and q-symmetral, q-symmetril for bimoulds.

Alternatively, we can first apply the evaluation map $\varphi : \mathbb{Q}\langle\mathcal{A}\rangle \to R$ for some commutative $\mathbb{Q}$-algebra R with unit to the generic diagonal series $\mathcal{W}(\mathcal{A})$.

Definition A.73. Let R be a commutative $\mathbb{Q}$-algebra with unit and $\varphi : \mathbb{Q}\langle\mathcal{A}\rangle \to R$ be a $\mathbb{Q}$-linear map. Define the (non-commutative) generating series with coefficients in R associated to φ by

$$\varphi(\mathcal{W}(\mathcal{A})) = \sum_{w\in\mathcal{A}^*} \varphi(w)w \in R\langle\langle\mathcal{A}\rangle\rangle.$$

Here $R\langle\langle\mathcal{A}\rangle\rangle$ denotes the completion of the space $R\langle\mathcal{A}\rangle = R \otimes \mathbb{Q}\langle\mathcal{A}\rangle$ with respect to the grading $\deg(a) = 1$ for all $a \in \mathcal{A}$.

Clearly, the generating series $\varphi(\mathcal{W}(\mathcal{A}))$ can also be decomposed into its homogeneous depth components $\varphi(\mathcal{W}(\mathcal{A}))_d$ for $d \geq 0$ (similar to Definition A.65).

Proposition A.74. *Let R be a commutative $\mathbb{Q}$-algebra with unit and $\varphi : \mathbb{Q}\langle\mathcal{A}\rangle \to R$ be a $\mathbb{Q}$-linear map. Assume that the algebra $(\mathbb{Q}\langle\mathcal{A}\rangle, *_\diamond)$ is graded with* $\deg(a) \geq 1$ *for all $a \in \mathcal{A}$, and denote by $\Delta_{*_\diamond}$ the dual coproduct to $*_\diamond$ with respect to the pairing given in* (A.60.1).

The map φ is an algebra morphism for the quasi-shuffle product $*_\diamond$ if and only if $\varphi(\mathcal{W}(\mathcal{A}))$ is grouplike for the coproduct $\Delta_{*_\diamond}$.

Proof. By Theorem A.61, we have $\Delta_{*_\diamond}\Big(\varphi(\mathcal{W}(\mathcal{A}))\Big) = \sum_{u,v\in\mathcal{A}^*} \varphi(u *_\diamond v)u \otimes v$. So φ is an algebra morphism for the quasi-shuffle product $*_\diamond$ if and only if

$$\Delta_{*_\diamond}\Big(\varphi(\mathcal{W}(\mathcal{A}))\Big) = \sum_{u,v\in\mathcal{A}^*} \varphi(u)\varphi(v)u \otimes v = \varphi(\mathcal{W}(\mathcal{A})) \otimes \varphi(\mathcal{W}(\mathcal{A})).$$

□

In particular, applying the map φ involves always a dualization process. This approach is the basis for Section 4.

A.5 Examples for generating series and quasi-shuffle algebras

In this subsection, we give explicit recursive formulas for several quasi-shuffle products on generating series of words (cf subsection A.4) for sake of reference.

Consider the alphabet $\mathcal{Y}^{\text{bi}} = \{y_{k,m} \mid k \geq 1,\ m \geq 0\}$ and let the depth of a word in $\mathbb{Q}\langle \mathcal{Y}^{\text{bi}} \rangle$ be given by

$$\operatorname{dep}(y_{k_1,m_1} \dots y_{k_d,m_d}) = d, \qquad k_1, \dots, k_d \geq 1,\ m_1, \dots, m_d \geq 0.$$

Define the $\mathbb{Q}$-linear map $\rho_{\mathcal{Y}^{\text{bi}}}$ by

$$\begin{aligned} \rho_{\mathcal{Y}^{\text{bi}}} : \mathbb{Q}\langle \mathcal{Y}^{\text{bi}} \rangle &\to \mathbb{Q}[X_1, Y_1, X_2, Y_2, \dots], \\ y_{k_1,m_1} \dots y_{k_d,m_d} &\mapsto X_1^{k_1-1} \frac{Y_1^{m_1}}{m_1!} \dots X_d^{k_d-1} \frac{Y_d^{m_d}}{m_d!}, \end{aligned}$$

then $\rho_{\mathcal{Y}^{\text{bi}}}$ essentially[8] satisfies the conditions in Definition A.64. The generating series of words in $\mathbb{Q}\langle \mathcal{Y}^{\text{bi}} \rangle$ associated to $\rho_{\mathcal{Y}^{\text{bi}}}$ is given by $\rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W})_0 = \mathbf{1}$ and

$$\rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W})_d \begin{pmatrix} X_1, \dots, X_d \\ Y_1, \dots, Y_d \end{pmatrix} = \sum_{\substack{k_1, \dots, k_d \geq 1 \\ m_1, \dots, m_d \geq 0}} y_{k_1,m_1} \dots y_{k_d,m_d} X_1^{k_1-1} \frac{Y_1^{m_1}}{m_1!} \dots X_d^{k_d-1} \frac{Y_d^{m_d}}{m_d!}, \quad d \geq 1.$$

First, we give a recursive formula for an arbitrary quasi-shuffle product $*_\diamond$ defined on $\mathbb{Q}\langle \mathcal{Y}^{\text{bi}} \rangle$ on the generating series of words.

Proposition A.75. *Let $(\mathbb{Q}\langle \mathcal{Y}^{\text{bi}} \rangle, *_\diamond)$ be a quasi-shuffle algebra. Then we have for all $0 < n < d$ that $\mathbf{1} *_\diamond \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W})_n = \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W})_n *_\diamond \mathbf{1} = \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W})_n$ and*

$$\begin{aligned} &\rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} *_\diamond \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix} \\ &= \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} \cdot \left(\rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_2, \dots, X_n \\ Y_2, \dots, Y_n \end{pmatrix} *_\diamond \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_{n+1}, \dots, X_d \\ Y_{n+1}, \dots, Y_d \end{pmatrix} \right) \\ &+ \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_{n+1} \\ Y_{n+1} \end{pmatrix} \cdot \left(\rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_1, \dots, X_n \\ Y_1, \dots, Y_n \end{pmatrix} *_\diamond \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_{n+2}, \dots, X_d \\ Y_{n+2}, \dots, Y_d \end{pmatrix} \right) \\ &+ \Big(\rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \diamond \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \Big) \begin{pmatrix} X_1, X_{n+1} \\ Y_1, Y_{n+1} \end{pmatrix} \cdot \left(\rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_2, \dots, X_n \\ Y_2, \dots, Y_n \end{pmatrix} *_\diamond \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \begin{pmatrix} X_{n+2}, \dots, X_d \\ Y_{n+2}, \dots, Y_d \end{pmatrix} \right), \end{aligned}$$

where

$$\Big(\rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \diamond \rho_{\mathcal{Y}^{\text{bi}}}(\mathcal{W}) \Big) \begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} = \sum_{\substack{k_1, k_2 \geq 1 \\ m_1, m_2 \geq 0}} (y_{k_1,m_1} \diamond y_{k_2,m_2}) X_1^{k_1-1} X_2^{k_2-1} \frac{Y_1^{m_1}}{m_1!} \frac{Y_2^{m_2}}{m_2!}.$$

Here $\cdot$ denotes the concatenation product (cf Proposition A.66).

[8] To be precisely in the situation of Definition A.64, we have to define the depth as $\operatorname{dep}(y_{k_1,m_1} \dots y_{k_d,m_d}) = 2d$. But this means the depth of every homogeneous element in $\mathbb{Q}\langle \mathcal{Y}^{\text{bi}} \rangle$ is divisible by 2, thus we stick to the above given depth map.

Proof. First, consider the case $d = 2$ and compute directly

$$\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1}{Y_1} *_\diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_2}{Y_2} = \sum_{\substack{k_1,k_2\geq 1\\ m_1,m_2\geq 0}} (y_{k_1,m_1} *_\diamond y_{k_2,m_2}) X_1^{k_1-1} X_2^{k_2-1} \frac{Y_1^{m_1}}{m_1!}\frac{Y_2^{m_2}}{m_2!}$$

$$= \sum_{\substack{k_1,k_2\geq 1\\ m_1,m_2\geq 0}} \Big(y_{k_1,m_1} y_{k_2,m_2} + y_{k_2,m_2} y_{k_1,m_1} + y_{k_1,m_1} \diamond y_{k_2,m_2}\Big) X_1^{k_1-1} X_2^{k_2-1} \frac{Y_1^{m_1}}{m_1!}\frac{Y_2^{m_2}}{m_2!}$$

$$= \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1, X_2}{Y_1, Y_2} + \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_2, X_1}{Y_2, Y_1} + \Big(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W}) \diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\Big)\binom{X_1, X_2}{Y_1, Y_2}.$$

Since the definition of the quasi-shuffle product $*_\diamond$ as well as the above formula for the generating series $\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})$ is recursive, the arbitrary depth case follows similarly by induction. □

Corollary A.76. *For all* $0 < n < d$, *one has* $\mathbf{1} \sqcup\!\sqcup\, \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n = \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n \sqcup\!\sqcup\, \mathbf{1} = \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n$ *and*

$$\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_\diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}$$
$$= \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1}{Y_1} \cdot \left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_2,\dots,X_n}{Y_2,\dots,Y_n} *_\diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}\right)$$
$$+ \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+1}}{Y_{n+1}} \cdot \left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_\diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+2},\dots,X_d}{Y_{n+2},\dots,Y_d}\right).$$

Proof. This is a direct consequence of Proposition A.75, since one obtains for the shuffle product that

$$\Big(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W}) \diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\Big)\binom{X_1, X_2}{Y_1, Y_2} = 0.$$

□

Corollary A.77. *For all* $0 < n < d$, *one obtains* $\mathbf{1} * \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n = \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n * \mathbf{1} = \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_n$ *and*

$$\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_\diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}$$
$$= \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1}{Y_1} \cdot \left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_2,\dots,X_n}{Y_2,\dots,Y_n} *_\diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}\right)$$
$$+ \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+1}}{Y_{n+1}} \cdot \left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_\diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+2},\dots,X_d}{Y_{n+2},\dots,Y_d}\right)$$
$$+ \frac{\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_1}{Y_1+Y_{n+1}} - \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+1}}{Y_1+Y_{n+1}}}{X_1 - X_{n+1}}$$
$$\cdot \left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_2,\dots,X_n}{Y_2,\dots,Y_n} * \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\binom{X_{n+2},\dots,X_d}{Y_{n+2},\dots,Y_d}\right).$$

Proof. Apply Proposition A.75 and observe that

$$\Big(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W}) \diamond \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\Big)\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} = \sum_{\substack{k_1,k_2\geq 1\\ m_1,m_2\geq 0}} y_{k_1+k_2,m_1+m_2} X_1^{k_1-1} X_2^{k_2-1} \frac{Y_1^{m_1}}{m_1!}\frac{Y_2^{m_2}}{m_2!}$$
$$= \frac{\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix} X_1 \\ Y_1+Y_2 \end{pmatrix} - \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix} X_2 \\ Y_1+Y_2 \end{pmatrix}}{X_1 - X_2}.$$

□

Next, consider the alphabet $\mathcal{B} = \{b_0, b_1, b_2, \ldots\}$ and let $\mathbb{Q}\langle\mathcal{B}\rangle^0$ the subalgebra of $\mathbb{Q}\langle\mathcal{B}\rangle$ spanned by all words, which do not start in b_0. The depth of a word in $\mathbb{Q}\langle\mathcal{B}\rangle^0$ is defined by

$$\mathrm{dep}(b_{k_1}b_0^{m_1}\ldots b_{k_d}b_0^{m_d}) = d, \qquad k_1,\ldots,k_d \geq 1,\ m_1,\ldots,m_d \geq 0.$$

Moreover, define the $\mathbb{Q}$-linear map $\rho_{\mathcal{B}}$ by

$$\rho_{\mathcal{B}}: \mathbb{Q}\langle\mathcal{B}\rangle^0 \to \mathbb{Q}[X_1,Y_1,X_2,Y_2,\ldots],$$
$$b_{k_1}b_0^{m_1}\ldots b_{k_d}b_0^{m_d} \mapsto X_1^{k_1-1}Y_1^{m_1}\ldots X_d^{k_d-1}Y_d^{m_d} \quad (k_1,\ldots,k_d\geq 1, m_1,\ldots,m_d\geq 0),$$

then $\rho_{\mathcal{B}}$ satisfies the conditions in Definition A.64. The generating series of words in $\mathbb{Q}\langle\mathcal{B}\rangle^0$ associated to $\rho_{\mathcal{B}}$ is given by $\rho_{\mathcal{B}}(\mathcal{W})_0 = \mathbf{1}$ and

$$\rho_{\mathcal{B}}(\mathcal{W})_d\begin{pmatrix} X_1,\ldots,X_d \\ Y_1,\ldots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\ldots,k_d\geq 1\\ m_1,\ldots,m_d\geq 0}} b_{k_1}b_0^{m_1}\ldots b_{k_d}b_0^{m_d} X_1^{k_1-1}Y_1^{m_1}\ldots X_d^{k_d-1}Y_d^{m_d}, \quad d\geq 1.$$

Proposition A.78. *(i) Let $(\mathbb{Q}\langle\mathcal{B}\rangle^0, ⧢)$ be the shuffle algebra, i.e., ⧢ is the quasi-shuffle product to $b_i \diamond b_j = 0$ for all $i,j\geq 0$ (Example A.53 1)). For all $0<n<d$, we obtain that $\mathbf{1} ⧢ \rho_{\mathcal{B}}(\mathcal{W})_n = \rho_{\mathcal{B}}(\mathcal{W})_n ⧢ \mathbf{1} = \rho_{\mathcal{B}}(\mathcal{W})_n$ and*

$$\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1,\ldots,X_n \\ Y_1,\ldots,Y_n \end{pmatrix} ⧢ \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1},\ldots,X_d \\ Y_{n+1},\ldots,Y_d \end{pmatrix}$$
$$= \left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1,\ldots,X_{n-1} \\ Y_1,\ldots,Y_{n-1} \end{pmatrix} ⧢ \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1},\ldots,X_d \\ Y_{n+1},\ldots,Y_d \end{pmatrix}\right)\cdot \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_n \\ Y_n+Y_d \end{pmatrix}$$
$$+ \left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1,\ldots,X_n \\ Y_1,\ldots,Y_n \end{pmatrix} ⧢ \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1},\ldots,X_{d-1} \\ Y_{n+1},\ldots,Y_{d-1} \end{pmatrix}\right)\cdot \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_d \\ Y_n+Y_d \end{pmatrix}.$$

(ii) Let $(\mathbb{Q}\langle\mathcal{B}\rangle^0, *_q)$ be the balanced quasi-shuffle algebra, i.e., $*_q$ is the quasi-shuffle product to $b_i \diamond_q b_j = \begin{cases} b_{i+j}, & i,j\geq 1 \\ 0 & \text{else} \end{cases}$ for all $i,j\geq 0$ (Example A.53 4)). For all $0<n<d$, we obtain $\mathbf{1} *_q \rho_{\mathcal{B}}(\mathcal{W})_n = \rho_{\mathcal{B}}(\mathcal{W})_n *_q \mathbf{1} = \rho_{\mathcal{B}}(\mathcal{W})_n$ and

$$\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1,\ldots,X_n \\ Y_1,\ldots,Y_n \end{pmatrix} *_q \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1},\ldots,X_d \\ Y_{n+1},\ldots,Y_d \end{pmatrix}$$
$$= \left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1,\ldots,X_{n-1} \\ Y_1,\ldots,Y_{n-1} \end{pmatrix} *_q \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1},\ldots,X_d \\ Y_{n+1},\ldots,Y_d \end{pmatrix}\right)\cdot \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_n \\ Y_n+Y_d \end{pmatrix}$$
$$+ \left(\rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_1,\ldots,X_n \\ Y_1,\ldots,Y_n \end{pmatrix} *_q \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_{n+1},\ldots,X_{d-1} \\ Y_{n+1},\ldots,Y_{d-1} \end{pmatrix}\right)\cdot \rho_{\mathcal{B}}(\mathcal{W})\begin{pmatrix} X_d \\ Y_n+Y_d \end{pmatrix}$$

$$+\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,\dots,X_{n-1}}{Y_1,\dots,Y_{n-1}} *_q \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+1},\dots,X_{d-1}}{Y_{n+1},\dots,Y_{d-1}}\right)$$
$$\cdot\frac{\rho_{\mathcal{B}}(\mathcal{W})\binom{X_n}{Y_n+Y_d}-\rho_{\mathcal{B}}(\mathcal{W})\binom{X_d}{Y_n+Y_d}}{X_n-X_d}.$$

Proof. We will only give a proof for (ii), part (i) follows from the same calculations modulo lower depth. Consider the case $d=2$. We obtain

$$\begin{aligned}\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} &= \sum_{\substack{k\geq 1\\ m\geq 0}} b_k b_0^m X_1^{k_1-1} Y_1^m,\\ &= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right)\cdot\frac{\mathbf{1}}{\mathbf{1}-b_0Y_1}, &\text{(A.78.1)}\\ &= \sum_{k\geq 1} b_k X_1^{k-1} + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot b_0Y_1. &\text{(A.78.2)}\end{aligned}$$

Hence we compute

$$\begin{aligned}
&\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} *_q \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\\
&= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_q \left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_q \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\cdot b_0Y_2\right)\\
&+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot b_0Y_1\right) *_q \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\\
&+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot b_0Y_1\right) *_q \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\cdot b_0Y_2\right)\\
&= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_q \left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \left(\left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_q \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2\right)\right)\cdot b_0\\
&+ \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\cdot b_0Y_2\cdot\sum_{k\geq 1} b_k X_1^{k-1} + \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1\right) *_q \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right)\cdot b_0\\
&+ \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot b_0Y_1\cdot\sum_{k\geq 1} b_k X_2^{k-1} + \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1\right) *_q \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\cdot b_0Y_2\right)\right)\cdot b_0\\
&+ \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot b_0Y_1\right) *_q \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2\right)\right)\cdot b_0\\
&= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_q \left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \left(\left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_q \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2\right)\right)\cdot b_0\\
&+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} - \sum_{k\geq 1} b_k X_2^{k_1}\right)\cdot\sum_{k\geq 1} b_k X_1^{k-1} + \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1\right) *_q \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right)\cdot b_0\\
&+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} - \sum_{k\geq 1} b_k X_1^{k-1}\right)\cdot\sum_{k\geq 1} b_k X_2^{k-1}
\end{aligned}$$

$$+\left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}Y_1\right)*_q\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}-\sum_{k\geq 1}b_kX_2^{k_1}\right)\right)\cdot b_0$$

$$+\left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}-\sum_{k\geq 1}b_kX_1^{k-1}\right)*_q\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}Y_2\right)\right)\cdot b_0$$

$$=\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)*_q\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)-2\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)\cdot\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)$$

$$+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\cdot\sum_{k\geq 1}b_kX_1^{k-1}+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot\sum_{k\geq 1}b_kX_2^{k-1}$$

$$+\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}*_q\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\right)\cdot b_0(Y_1+Y_2)$$

where the first equality is obtained from (A.78.2), the second equality is just an application of the definition of $*_q$, the third equality again follows from (A.78.2) and the fourth equality is a simple cancellation and reordering. Therefore, we obtain

$$\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}*_q\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} \qquad \text{(A.78.3)}$$

$$=\frac{\mathbf{1}}{\mathbf{1}-b_0(Y_1+Y_2)}\cdot\Bigg(\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)*_q\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)-2\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)\cdot\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)$$

$$+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\cdot\sum_{k\geq 1}b_kX_1^{k-1}+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot\sum_{k\geq 1}b_kX_2^{k-1}\Bigg)$$

$$=\frac{\mathbf{1}}{\mathbf{1}-b_0(Y_1+Y_2)}\cdot\Bigg(\left(\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)*_q\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)-2\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)\cdot\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)\right)$$

$$+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\cdot\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1+Y_2}+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_1+Y_2}\Bigg)$$

$$=\frac{\mathbf{1}}{\mathbf{1}-b_0(Y_1+Y_2)}\cdot\Bigg(\left(\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)*_q\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)-2\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)\cdot\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)\right)$$

$$+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2,X_1}{Y_2,Y_1+Y_2}+\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,X_2}{Y_1,Y_1+Y_2}\Bigg),$$

here the second equality is obtained from (A.78.1) and the third equality follows from applying the concatenation product (A.66). Moreover, one verifies by applying the definition of $*_q$ and some power series manipulation

$$\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)*_q\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)$$

$$=2\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)\cdot\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)+\sum_{k_1,k_2\geq 1}b_{k_1+k_2}X_1^{k_1-1}X_2^{k_2-1}$$

$$=2\left(\sum_{k\geq 1}b_kX_1^{k-1}\right)\cdot\left(\sum_{k\geq 1}b_kX_2^{k-1}\right)+\frac{\sum_{k\geq 1}b_kX_1^{k_1}-\sum_{k\geq 1}b_kX_2^{k-1}}{X_1-X_2}$$

Applying this result to (A.78.3), we obtain together with (A.78.1)

$$
\begin{aligned}
&\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} *_q \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} \\
&= \frac{\mathbf{1}}{\mathbf{1} - b_0(Y_1+Y_2)} \cdot \left(\frac{\sum_{k\geq 1} b_k X_1^{k_1} - \sum_{k\geq 1} b_k X_2^{k-1}}{X_1 - X_2}\right) + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2, X_1}{Y_2, Y_1+Y_2} \\
&\quad + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1, X_2}{Y_1, Y_1+Y_2} \\
&= \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2, X_1}{Y_2, Y_1+Y_2} + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1, X_2}{Y_1, Y_1+Y_2} + \frac{\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1+Y_2} - \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_1+Y_2}}{X_1 - X_2},
\end{aligned}
$$

which equals exactly the claimed formula of $*_q$ for the generating series in depth 2. Since the definition of the product $*_q$ and the above generating series formula are both recursive (and any quasi-shuffle product can be equally defined from the left and the right), we obtain the desired formula in arbitrary depth by applying induction and the same computations as before. □

Proposition A.79. *Let* $(\mathbb{Q}\langle\mathcal{B}\rangle^0, *_{\mathrm{SZ}})$ *be the SZ stuffle algebra, i.e.,* $*_{\mathrm{SZ}}$ *is the quasi-shuffle product to* $b_i \diamond_{\mathrm{SZ}} b_j = b_{i+j}$ *for all* $i, j \geq 0$ *(Example A.53 3)). We have for all* $0 < n < d$ *that* $\mathbf{1} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})_n = \rho_{\mathcal{B}}(\mathcal{W})_n *_{\mathrm{SZ}} \mathbf{1} = \rho_{\mathcal{B}}(\mathcal{W})_n$ *and*

$$
\begin{aligned}
&\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d} \\
&= (Y_n+\mathbf{1})\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,\dots,X_{n-1}}{Y_1,\dots,Y_{n-1}} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+1},\dots,X_d}{Y_{n+1},\dots,Y_d}\right) \\
&\qquad\qquad \cdot \rho_{\mathcal{B}}(\mathcal{W})\binom{X_n}{(Y_n+1)(Y_d+1)-1} \\
&\quad + (Y_n+\mathbf{1})\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,\dots,X_n}{Y_1,\dots,Y_n} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+1},\dots,X_{d-1}}{Y_{n+1},\dots,Y_{d-1}}\right) \\
&\qquad\qquad \cdot \rho_{\mathcal{B}}(\mathcal{W})\binom{X_d}{(Y_n+1)(Y_d+1)-1} \\
&\quad + \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1,\dots,X_{n-1}}{Y_1,\dots,Y_{n-1}} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})\binom{X_{n+1},\dots,X_{d-1}}{Y_{n+1},\dots,Y_{d-1}}\right) \\
&\qquad\qquad \cdot \frac{\rho_{\mathcal{B}}(\mathcal{W})\binom{X_n}{(Y_n+1)(Y_d+1)-1} - \rho_{\mathcal{B}}(\mathcal{W})\binom{X_d}{(Y_n+1)(Y_d+1)-1}}{X_n - X_d}.
\end{aligned}
$$

Proof. First, restrict to the case $d = 2$. We obtain

$$
\begin{aligned}
\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} &= \sum_{\substack{k\geq 1\\ m\geq 0}} b_k b_0^m X_1^{k_1-1} Y_1^m \\
&= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) \cdot \frac{\mathbf{1}}{\mathbf{1} - b_0 Y_1} \qquad \text{(A.79.1)}
\end{aligned}
$$

$$= \sum_{k\geq 1} b_k X_1^{k-1} + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} \cdot b_0 Y_1. \tag{A.79.2}$$

Then, calculate

$$\begin{aligned}
&\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} \\
&= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} \cdot b_0 Y_2\right) \\
&+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} \cdot b_0 Y_1\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right) \\
&+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} \cdot b_0 Y_1\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} \cdot b_0 Y_2\right) \\
&= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \left(\left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2\right)\right) \cdot b_0 \\
&+ \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} \cdot b_0 Y_2 \cdot \sum_{k\geq 1} b_k X_1^{k-1} + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2 \cdot \sum_{k\geq 1} b_k X_1^{k-1} \\
&+ \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right) \cdot b_0 + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} \cdot b_0 Y_1 \cdot \sum_{k\geq 1} b_k X_2^{k-1} \\
&+ \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1 \cdot \sum_{k\geq 1} b_k X_2^{k-1} + \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} \cdot b_0 Y_2\right)\right) \cdot b_0 \\
&+ \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} \cdot b_0 Y_1\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2\right)\right) \cdot b_0 \\
&+ \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2\right)\right) \cdot b_0 \\
&= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \left(\left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2\right)\right) \cdot b_0 \\
&+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} - \sum_{k\geq 1} b_k X_2^{k_1}\right) \cdot \sum_{k\geq 1} b_k X_1^{k-1} + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2 \cdot \sum_{k\geq 1} b_k X_1^{k-1} \\
&+ \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right) \cdot b_0 \\
&+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} - \sum_{k\geq 1} b_k X_1^{k-1}\right) \cdot \sum_{k\geq 1} b_k X_2^{k-1} + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1 \cdot \sum_{k\geq 1} b_k X_2^{k-1} \\
&+ \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} Y_1\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} - \sum_{k\geq 1} b_k X_2^{k_1}\right)\right) \cdot b_0 \\
&+ \left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} - \sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} Y_2\right)\right) \cdot b_0
\end{aligned}$$

$$+\left(\left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}Y_1\right) *_{\mathrm{SZ}} \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}Y_2\right)\right)\cdot b_0$$

$$= \left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right) - 2\left(\sum_{k\geq 1} b_k X_1^{k-1}\right)\cdot\left(\sum_{k\geq 1} b_k X_2^{k-1}\right)$$

$$+ \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}(\mathbf{1}+Y_2)\cdot\sum_{k\geq 1} b_k X_1^{k-1} + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}(\mathbf{1}+Y_1)\cdot\sum_{k\geq 1} b_k X_2^{k-1}$$

$$+ \left(\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\right)\cdot b_0(Y_1+Y_2+Y_1Y_2),$$

where the first equality follows from (A.79.2), the second equality is obtained from the definition of $*_q$, the third equality again follows from (A.79.2) and the fourth equality is just cancellation and reordering. We deduce

$$\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2} \tag{A.79.3}$$

$$= \frac{\mathbf{1}}{\mathbf{1}-b_0(Y_1+Y_2+Y_1Y_2)}\cdot\left(\left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right.$$

$$- 2\left(\sum_{k\geq 1} b_k X_1^{k-1}\right)\cdot\left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}(\mathbf{1}+Y_2)\cdot\sum_{k\geq 1} b_k X_1^{k-1}$$

$$\left.+ \rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}(\mathbf{1}+Y_1)\cdot\sum_{k\geq 1} b_k X_2^{k-1}\right)$$

$$= \frac{\mathbf{1}}{\mathbf{1}-b_0(Y_1+Y_2+Y_1Y_2)}\cdot\left(\left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right.$$

$$\left.- 2\left(\sum_{k\geq 1} b_k X_1^{k-1}\right)\cdot\left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right) + (\mathbf{1}+Y_2)\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}\cdot\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1+Y_2+Y_1Y_2}$$

$$+ (\mathbf{1}+Y_1)\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1}\cdot\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_1+Y_2+Y_1Y_2}$$

$$= \frac{\mathbf{1}}{\mathbf{1}-b_0(Y_1+Y_2+Y_1Y_2)}\cdot\left(\left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right.$$

$$\left.- 2\left(\sum_{k\geq 1} b_k X_1^{k-1}\right)\cdot\left(\sum_{k\geq 1} b_k X_2^{k-1}\right)\right) + (\mathbf{1}+Y_2)\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2, X_1}{Y_2, (Y_1+1)(Y_2+1)-1}$$

$$+ (\mathbf{1}+Y_1)\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1, X_2}{Y_1, (Y_1+1)(Y_2+1)-1},$$

here the second equality follows from (A.79.1) and the third equality is obtained from applying the concatenation product (A.66). Moreover, one verifies by applying the definition of $*_{\mathrm{SZ}}$ and some power series manipulation

$$\left(\sum_{k\geq 1} b_k X_1^{k-1}\right) *_{\mathrm{SZ}} \left(\sum_{k\geq 1} b_k X_2^{k-1}\right)$$

$$= 2\left(\sum_{k\geq 1} b_k X_1^{k-1}\right)\cdot\left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \sum_{k_1,k_2\geq 1} b_{k_1+k_2} X_1^{k_1-1}X_2^{k_2-1}$$

$$= 2\left(\sum_{k\geq 1} b_k X_1^{k-1}\right)\cdot\left(\sum_{k\geq 1} b_k X_2^{k-1}\right) + \frac{\sum_{k\geq 1} b_k X_1^{k_1} - \sum_{k\geq 1} b_k X_2^{k-1}}{X_1 - X_2}$$

Inserting this formula into (A.79.3), one obtains together with (A.79.1)

$$\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{Y_1} *_{\mathrm{SZ}} \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{Y_2}$$

$$= \frac{\mathbf{1}}{\mathbf{1} - b_0(Y_1+Y_2+Y_1Y_2)}\cdot\left(\frac{\sum_{k\geq 1} b_k X_1^{k_1} - \sum_{k\geq 1} b_k X_2^{k-1}}{X_1 - X_2}\right)$$

$$+ (\mathbf{1}+Y_2)\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2, X_1}{Y_2, (Y_1+1)(Y_2+1)-1} + (\mathbf{1}+Y_1)\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1, X_2}{Y_1, (Y_1+1)(Y_2+1)-1}$$

$$= (\mathbf{1}+Y_2)\rho_{\mathcal{B}}(\mathcal{W})\binom{X_2, X_1}{Y_2, (Y_1+1)(Y_2+1)-1} + (\mathbf{1}+Y_1)\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1, X_2}{Y_1, (Y_1+1)(Y_2+1)-1}$$

$$+ \frac{\rho_{\mathcal{B}}(\mathcal{W})\binom{X_1}{(Y_1+1)(Y_2+1)-1} - \rho_{\mathcal{B}}(\mathcal{W})\binom{X_2}{(Y_1+1)(Y_2+1)-1}}{X_1 - X_2},$$

which is exactly the formula for the generating series $\rho_{\mathcal{B}}(\mathcal{W})$ in depth 2. Since both the above generating series formula and the SZ stuffle product are defined recursively (and each quasi-shuffle product can be equally defined recursively from the left and the right), we obtain the claim in arbitrary depths by applying induction and the same arguments as before. □

A.6 Affine group schemes

We give a rough introduction to affine group schemes in this subsection. More details and missing proofs can be found in [DG70], [Mil17], [Rac00, I.4], and [Wa79].

Definition A.80. Let $\mathbf{C}$ be a locally small category. A functor $F : \mathbf{C} \to \mathrm{Sets}$ is called representable if there is an object $A \in \mathbf{C}$, such that F is naturally isomorphic to the Hom-functor

$$\begin{aligned} \mathrm{Hom}_{\mathbf{C}}(A, -) : \mathbf{C} &\to \mathrm{Sets}, \\ B &\mapsto \mathrm{Hom}_{\mathbf{C}}(A, B). \end{aligned}$$

In this case, one says that A represents the functor F.

Let $\mathbb{Q}$-Alg be the category of commutative $\mathbb{Q}$-algebras with unit (we require an algebra to be associative by definition).
An affine scheme is a representable functor $F : \mathbb{Q}\text{-Alg} \to \mathrm{Sets}$.

Theorem A.81. *(Yoneda's Lemma) Let $\mathbf{C}$ be a locally small category and $E, F : \mathbf{C} \to$ Sets be two functors represented by A, B. Then any natural transformation $\Phi : E \to F$ corresponds uniquely to a morphism $\varphi : B \to A$ in $\mathbf{C}$.* □

Let $\Phi : E \to F$ be some natural transformation. Apply the map $\Phi(A) : E(A) \to F(A)$ to $\mathrm{id} : A \to A \in \mathrm{Hom}_{\mathbf{C}}(A, A) \simeq E(A)$ to obtain a morphism $\varphi : B \to A \in \mathrm{Hom}_{\mathbf{C}}(B, A) \simeq F(A)$. Then φ is exactly the morphism corresponding to Φ in the previous theorem.

Definition A.82. An affine group scheme is a representable functor $G : \mathbb{Q}\text{-Alg} \to \mathrm{Groups}$.

Let $G : \mathbb{Q}\text{-Alg} \to \mathrm{Groups}$ be an affine group scheme represented by A. Then there are natural transformations

$$\mathrm{mult} : G \times G \to G, \quad \mathrm{unit} : \{e\} \to G, \quad \mathrm{inv} : G \to G$$

corresponding to the group multiplication, the unit, and the inverse elements. Here we denote by $\{e\}$ the functor $\mathbb{Q}\text{-Alg} \to \mathrm{Groups}$ mapping any $\mathbb{Q}$-algebra R to the trivial group with one element. By Theorem A.81 the above three natural transformations correspond to algebra morphisms

$$\Delta : A \to A \otimes A, \quad \varepsilon : A \to \mathbb{Q}, \quad S : A \to A.$$

Here the associativity of the group multiplication translates into the coassociativity of Δ (cf Definition A.16), the unit property translates into the counit property of ε and Δ (cf Definition A.16), and the inverse elements property translates into the antipode property of S (cf Definition A.29). Thus, the maps Δ, ε and S equip the algebra A with a Hopf algebra structure. Summarizing the previous observations leads to the following.

Theorem A.83. *([Wa79, Subsection 1.4]) Affine group schemes are in one-to-one correspondence to commutative Hopf algebras over $\mathbb{Q}$.* □

Example A.84. For each commutative $\mathbb{Q}$-algebra R with unit, consider the dual quasi-shuffle Hopf algebra $(R\langle\langle \mathcal{A} \rangle\rangle, \mathrm{conc}, \Delta_{*_\diamond})$ obtained in Theorem A.61. The functor

$$\begin{aligned} F : \mathbb{Q}\text{-Alg} &\to \mathrm{Sets}, \\ R &\mapsto R\langle\langle \mathcal{A} \rangle\rangle \end{aligned}$$

is an affine scheme represented by the polynomial algebra $\mathbb{Q}[(z_w)_{w\in\mathcal{A}^*}]$, since there are natural bijections

$$R\langle\langle\mathcal{A}\rangle\rangle \to \mathrm{Hom}_{\mathbb{Q}\text{-Alg}}\Big(\mathbb{Q}[(z_w)_{w\in\mathcal{A}^*}], R\Big),$$
$$\Phi \mapsto \Big(z_w \mapsto (\Phi \mid w)\Big).$$

Here $(\Phi \mid w)$ denotes the coefficient of Φ in w. The grouplike elements $\mathrm{Grp}(R\langle\langle\mathcal{A}\rangle\rangle)$ for the coproduct $\Delta_{*_\diamond}$ form a group with the concatenation product (Theorem A.38). Hence restricting the images of the affine scheme F to the grouplike elements $\mathrm{Grp}(R\langle\langle\mathcal{A}\rangle\rangle)$, one obtains an affine group scheme

$$G : \mathbb{Q}\text{-Alg} \to \text{Groups},$$
$$R \mapsto \mathrm{Grp}(R\langle\langle\mathcal{A}\rangle\rangle).$$

By the duality given in Theorem A.61, the affine group scheme G is represented by

$$B = \mathbb{Q}[(z_w)_{w\in\mathcal{A}^*}] \Big/ \Big\langle z_u z_v - z_{u *_\diamond v} \mid u, v \in \mathcal{A}^* \Big\rangle,$$

where we set $z_{\lambda u+\mu v} := \lambda z_u + \mu z_v$ for $u, v \in \mathcal{A}^*$, $\lambda, \mu \in R$. By Theorem A.83, B is a Hopf algebra. Again by the duality in Theorem A.61, the coproduct on B is given by

$$\Delta(z_w) = \sum_{uv=w} z_u \otimes z_v, \qquad w \in \mathcal{A}^*.$$

Definition A.85. An affine (group) scheme G represented by A is called algebraic if A is a finitely generated algebra.

For an affine group scheme, one uses the additional Hopf algebra structure on the representing algebra to obtain the following.

Theorem A.86. *Any affine group scheme is an inverse limit of algebraic affine group schemes.* □

Example A.87. Let V be a finite-dimensional $\mathbb{Q}$-vector space. Then there is an algebraic affine group scheme

$$\mathbb{A}^V : \mathbb{Q}\text{-Alg} \to \text{Groups},$$
$$R \mapsto (V \otimes_{\mathbb{Q}} R, +)$$

represented by the symmetric algebra $\mathcal{S}(V^*)$. More generally, let V be a complete filtered $\mathbb{Q}$-vector space (Definition A.44), such that the quotients $\mathrm{Fil}^{(j)} V \big/ \mathrm{Fil}^{(j+1)} V$ are finite-dimensional for all $j \geq 0$ and $\bigcap_{j\geq 0} \mathrm{Fil}^{(j)} V = \{0\}$. Then the functor

$$\widehat{\mathbb{A}}^V : \mathbb{Q}\text{-Alg} \to \text{Groups},$$
$$R \mapsto (V \hat{\otimes}_{\mathbb{Q}} R, +)$$

satisfies $\widehat{\mathbb{A}}^V = \varprojlim \mathbb{A}^{\mathrm{Fil}^{(j)} V / \mathrm{Fil}^{(j+1)} V}$. Thus, $\widehat{\mathbb{A}}^V$ is an affine group scheme represented by the algebra

$$\varinjlim \mathcal{S}\Big(\Big(\mathrm{Fil}^{(j)} V \big/ \mathrm{Fil}^{(j+1)} V\Big)^*\Big) = \mathcal{S}\Big(\varinjlim \Big(\mathrm{Fil}^{(j)} V \big/ \mathrm{Fil}^{(j+1)} V\Big)^*\Big) = \mathcal{S}(\mathrm{gr}\, V^\vee),$$

where the associated graded space $\mathrm{gr}\, V$ is introduced in Definition A.48 and the graded dual $\mathrm{gr}\, V^\vee$ is defined in Example A.19.

Similar to the connection of Lie groups and Lie algebras, one can assign a Lie algebra functor to each affine group scheme.

Definition A.88. For any commutative $\mathbb{Q}$-algebra R with unit, let $R[\varepsilon] = {}^{R[t]}\!/\!_{\langle t^2 \rangle}$ be the algebra of dual numbers over R, so $\varepsilon^2 = 0$. For an affine group scheme G, define the Lie algebra functor as

$$\begin{aligned} g : \mathbb{Q}\text{-Alg} &\to \text{Lie-Alg}, \\ R &\mapsto \ker\Big(G(R[\varepsilon] \twoheadrightarrow R)\Big). \end{aligned}$$

Here $R[\varepsilon] \twoheadrightarrow R$ denotes the canonical projection induced by $\varepsilon \mapsto 0$.

In particular, $g(R)$ consists of all elements in $G(R[\varepsilon])$ of the form $1 + \varepsilon x$. Thus, in all examples occurring in this work we will identify

$$g(R) = \{x \mid 1 + \varepsilon x \in G(R[\varepsilon])\}.$$

Proposition A.89. *Let G be an affine group scheme represented by a graded Hopf algebra H and denote by g the Lie algebra functor to G. Then one has*

$$g(\mathbb{Q}) \simeq \mathrm{Q}(H)^\vee,$$

where $\mathrm{Q}(H)^\vee$ denotes the graded dual of the space of indecomposables of H (Definition A.41, Example A.19 (ii)). □

If the affine group scheme G is algebraic, then $g(\mathbb{Q})$ is finite-dimensional and one obtains $g(R) = g(\mathbb{Q}) \otimes R$ for any commutative $\mathbb{Q}$-algebra R with unit. By Theorem A.86 any affine group scheme G is an inverse limit $G = \varprojlim G_n$, where the G_n are algebraic affine group schemes. Therefore, we have for each commutative $\mathbb{Q}$-algebra R with unit

$$g(R) = \varprojlim g_n(R) = \varprojlim \Big(g_n(\mathbb{Q}) \otimes R\Big) = g(\mathbb{Q}) \otimes R.$$

Identifying $g(\mathbb{Q})$ with the space of all derivations on the representing Hopf algebra of G, which are left-invariant under the coproduct, gives the Lie bracket on $g(\mathbb{Q})$. Via the identification $g(R) = g(\mathbb{Q}) \otimes R$, one obtains the Lie bracket on each space $g(R)$.

Proposition A.90. *Let G be an affine group scheme. Then the Lie algebra functor $g : \mathbb{Q}\text{-Alg} \to \text{Lie-Alg}$ is an affine scheme represented by the algebra $\mathcal{S}(\operatorname{gr} g(\mathbb{Q})^\vee)$.*

Sketch of proof. If G is algebraic, then $g(\mathbb{Q})$ is finite-dimensional and $g(R) = g(\mathbb{Q}) \otimes R$. In particular, the functor g is equal to the functor $\mathbb{A}^{g(\mathbb{Q})}$ given in Example A.87 and thus represented by $\mathcal{S}(g(\mathbb{Q})^*)$.
By Theorem A.86 any affine group scheme G is an inverse limit $G = \varprojlim G_n$, where the G_n are algebraic affine group schemes. Therefore, $g(\mathbb{Q}) = \varprojlim g_n(\mathbb{Q})$ is a complete filtered vector space. Since $g(R) = g(\mathbb{Q}) \hat{\otimes} R$, the functor g is equal to $\widehat{\mathbb{A}}^{g(\mathbb{Q})}$. So by Example A.87 g is represented by the algebra $\mathcal{S}(\operatorname{gr} g(\mathbb{Q})^\vee)$. □

Next, we introduce an important class of affine group schemes, for which there exists a natural isomorphism to their Lie algebra functors.

Definition A.91. For a $\mathbb{Q}$-vector space V, define the functor $\mathrm{Gl}(V)$ by

$$\begin{aligned} \mathrm{Gl}(V) : \mathbb{Q}\text{-Alg} &\to \text{Groups}, \\ R &\mapsto \mathrm{Aut}_R(V \otimes R). \end{aligned}$$

A linear representation of an affine group scheme G on a $\mathbb{Q}$-vector space V is a natural transformation $\rho : G \to \mathrm{Gl}(V)$. Such a linear representation $\rho : G \to \mathrm{Gl}(V)$ of G is called faithful if for any commutative $\mathbb{Q}$-algebra R with unit the map $\rho(R) : G(R) \to \mathrm{Gl}(V)(R)$ is injective.

If V is a finite-dimensional vector space, then $\mathrm{Gl}(V)$ is an affine group scheme.

Definition A.92. An algebraic affine group scheme G is called unipotent if there is a faithful linear representation $\rho : G \to \mathrm{Gl}(V)$ on some finite-dimensional $\mathbb{Q}$-vector space V, such that the following holds

- V contains a finite flag $V = V_0 \supseteq V_1 \supseteq V_2 \supseteq \cdots \supseteq V_n = \{0\}$.
- For each commutative $\mathbb{Q}$-algebra R with unit and $i = 1, \dots, n$, the subspace $V_i \otimes R$ is invariant under the action of $G(R)$, i.e., $\rho(R)(G(R))(V_i \otimes R) \subseteq V_i \otimes R$.
- For any commutative $\mathbb{Q}$-algebra R with unit, the action of $G(R)$ on $\left(V_i / V_{i+1} \right) \otimes R$ is trivial.

An arbitrary affine group scheme is called pro-unipotent if it is an inverse limit of unipotent algebraic affine group schemes.

Proposition A.93. *Let G be an affine group scheme with Lie algebra functor g. For any commutative $\mathbb{Q}$-algebra R with unit and $x \in g(R)$, there is a unique element* $\exp(tx) \in G(R[[t]])$*, such that*

(i) $\exp(\varepsilon x) = x$ *in* $G(R[\varepsilon])$*,*

(ii) $\exp(tx)\exp(t'x) = \exp((t+t')x)$ *in* $G(R[[t,t']])$*,*

(iii) $\exp(tx)\exp(ty) = \exp(t(x+y))$ *if* $x, y \in G(R)$ *commute.*

□

Example A.94. Let V be a finite-dimensional vector space and consider the affine group scheme $\mathrm{Gl}(V)$. The corresponding Lie algebra functor is given by

$$\begin{aligned} \mathrm{gl}(V) : \mathbb{Q}\text{-Alg} &\to \text{Lie-Alg}, \\ R &\mapsto \mathrm{End}_R(V \otimes R), \end{aligned}$$

where the Lie bracket on the sets $\mathrm{End}_R(V \otimes R)$ is simply the commutator. For each commutative $\mathbb{Q}$-algebra R with unit and $f \in \mathrm{gl}(V)(R)$, one has

$$\exp(tf) = \sum_{i \geq 0} \frac{t^i f^i}{i!} \text{ in } \mathrm{Gl}(V)(R[[t]]).$$

One simply checks that the element $\sum_{i \geq 0} \frac{t^i f^i}{i!}$ satisfies (i)-(iii) in Proposition A.93, then the claim follows from the uniqueness.

Let G be a unipotent algebraic affine group scheme with Lie algebra functor g. Then it can be shown that for each commutative $\mathbb{Q}$-algebra R with unit and each $x \in g(R)$, the element $\exp(tx)$ is contained in $G(R[t])$. In particular, one can specialize in $t = 1$ and obtains maps

$$g(R) \to G(R), \quad x \mapsto \exp(x).$$

One verifies that these maps possess inverses and the construction is functorial. Thus, by passing to inverse limits, the following is obtained.

Theorem A.95. *([DG70, IV, Proposition 4.1]) Let G be a pro-unipotent affine group scheme with Lie algebra functor g. Then there is a natural isomorphism*

$$\exp : g \to G.$$

□

The Baker-Campbell-Hausdorff series ([Mil17, p. 260]) gives the explicit relation between the Lie bracket on g and the group multiplication on G under the isomorphism exp.

Example A.96. In Example A.84 we considered the dual quasi-shuffle Hopf algebra $(R\langle\langle\mathcal{A}\rangle\rangle, \mathrm{conc}, \Delta_{*_\diamond})$ (where the unit was denoted by $\mathbf{1}$) and obtained the corresponding affine group scheme

$$\begin{aligned} G : \mathbb{Q}\text{-Alg} &\to \text{Groups}, \\ R &\mapsto \mathrm{Grp}(R\langle\langle\mathcal{A}\rangle\rangle). \end{aligned}$$

Let g be the Lie algebra functor to G. By definition for each commutative $\mathbb{Q}$-algebra R with unit, the set $g(R)$ consists of all $\Psi \in R\langle\langle\mathcal{A}\rangle\rangle$, such that $\mathbf{1} + \varepsilon\Psi \in G(R[\varepsilon])$. Compute for $\mathbf{1} + \varepsilon\Psi \in G(R[\varepsilon])$

$$\begin{aligned} \mathbf{1} \otimes \mathbf{1} + \varepsilon\Delta_{*_\diamond}(\Psi) = \Delta_{*_\diamond}(\mathbf{1} + \varepsilon\Psi) &= \big(\mathbf{1} + \varepsilon\Psi\big) \otimes \big(\mathbf{1} + \varepsilon\Psi\big) \\ &= \mathbf{1} \otimes \mathbf{1} + \mathbf{1} \otimes \varepsilon\Psi + \varepsilon\Psi \otimes \mathbf{1} + \varepsilon\Psi \otimes \varepsilon\Psi \\ &= \mathbf{1} \otimes \mathbf{1} + \varepsilon\Big(\mathbf{1} \otimes \Psi + \Psi \otimes \mathbf{1}\Big). \end{aligned}$$

Thus $g(R)$ consists of the primitive elements for $\Delta_{*_\diamond}$, this means for each commutative $\mathbb{Q}$-algebra R with unit we have

$$g(R) = \mathrm{Prim}(R\langle\langle\mathcal{A}\rangle\rangle).$$

We want to derive the Lie bracket $[-,-]_g$ on $g(R)$ from the group multiplication on $G(R)$, which is the concatenation product. For each commutative $\mathbb{Q}$-algebra R with unit and $\Phi \in G(R)$, define the map

$$\sigma_R(\Phi) : R\langle\langle\mathcal{A}\rangle\rangle \to R\langle\langle\mathcal{A}\rangle\rangle, \Phi' \mapsto \Phi\Phi'.$$

Moreover, for $\Psi \in g(R)$ define the morphism $s_R(\Psi) : R\langle\langle\mathcal{A}\rangle\rangle \to R\langle\langle\mathcal{A}\rangle\rangle$ by

$$\sigma_R(\mathbf{1} + \varepsilon\Psi) = \mathrm{id} + \varepsilon s_R(\Psi).$$

Since $s_R : (g(R), [-,-]_g) \to (\mathrm{End}(R\langle\langle\mathcal{A}\rangle\rangle), [-,-])$ is the Lie algebra morphism deduced from the group morphism $\sigma_R : (G(R), \mathrm{conc}) \to (\mathrm{Aut}(R\langle\langle\mathcal{A}\rangle\rangle), \circ)$, one obtains

$$s_R([\Psi_1, \Psi_2]_g) = [s_R(\Psi_1), s_R(\Psi_2)], \qquad \Psi_1, \Psi_2 \in g(R). \tag{A.96.1}$$

For $\mathbf{1} + \varepsilon\Psi \in G(R[\varepsilon])$, compute

$$\mathbf{1} + \varepsilon\Psi = \sigma_R(\mathbf{1} + \varepsilon\Psi)(\mathbf{1}) = \mathbf{1} + \varepsilon s_R(\Psi)(\mathbf{1})$$

and thus $s_R(\Psi)(\mathbf{1}) = \Psi$. Applying this to (A.96.1) gives

$$[\Psi_1, \Psi_2]_g = s_R(\Psi_1)(\Psi_2) - s_R(\Psi_2)(\Psi_1), \qquad \Psi_1, \Psi_2 \in g(R). \tag{A.96.2}$$

For $\mathbf{1} + \varepsilon\Psi \in G(R[\varepsilon])$ and each $x \in R\langle\langle\mathcal{A}\rangle\rangle$, compute

$$x + \varepsilon s_R(\Psi)(x) = \sigma_R(\mathbf{1} + \varepsilon\Psi)(x) = (\mathbf{1} + \varepsilon\Psi)x = x + \varepsilon\Psi x$$

and thus $s_R(\Psi)(x) = \Psi x$. Inserting this into the equation (A.96.2) yields

$$[\Psi_1, \Psi_2]_g = \Psi_1\Psi_2 - \Psi_2\Psi_1.$$

Thus for each commutative $\mathbb{Q}$-algebra R with unit, the Lie bracket on $g(R) = \mathrm{Prim}(R\langle\langle\mathcal{A}\rangle\rangle)$ is exactly the commutator with respect to the concatenation (cf. Theorem A.38).

Moreover, one can show that G is pro-unipotent. So by Theorem A.95, one obtains a natural isomorphism

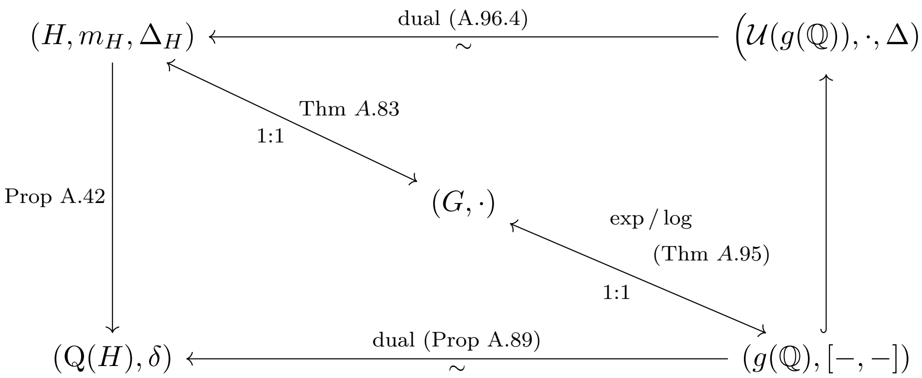
$$\exp : g \to G.$$

Explicitly, for each commutative $\mathbb{Q}$-algebra R with unit, this isomorphism is given by (cf. Theorem A.51)

$$\exp(R) : \mathrm{Grp}(R\langle\langle\mathcal{A}\rangle\rangle) \to \mathrm{Prim}(R\langle\langle\mathcal{A}\rangle\rangle),$$
$$\Psi \mapsto \exp(R)(\Psi) = \sum_{i\geq 0} \frac{1}{i!}\Psi^i,$$

where Ψ^i denotes the i-times concatenation of the element Ψ.

We summarize some important results of this section. Let $(G, \cdot)$ be a pro-unipotent affine group scheme, such that the corresponding Hopf algebra (H, m_H, Δ_H) (cf Theorem A.83) is graded, commutative and satisfies rank $H^{(0)} = 1$. Moreover, let g be the Lie algebra functor associated to G (Definition A.88). Then there is the following diagram



(A.96.3)

The upper duality is obtained from Theorem A.39, A.43, and Proposition A.89

$$H^\vee \simeq \mathcal{U}(\mathrm{Prim}(H^\vee)) \simeq \mathcal{U}(\mathrm{Q}(H)^\vee) \simeq \mathcal{U}(g(\mathbb{Q})). \tag{A.96.4}$$

Appendix B Multiple zeta values and Lie algebras

This section starts with a short basic introduction to the theory of multiple zeta values. Then we will present two different approaches obtaining Lie algebras related to multiple zeta values. On the one hand, there is the approach via non-commutative power series ([Rac00]), which shows that the algebra of formal multiple zeta values is a free polynomial algebra. On the other hand, there is the commutative approach via moulds ([Ec11],[Sc15]), which deals with the usual generating series of multiple zeta values. We will end this section by comparing the Lie algebras obtained in these two different ways.

B.1 The algebra of multiple zeta values

We introduce the algebra of multiple zeta values and explain shortly the extended double shuffle relation between multiple zeta values. For details, we refer to [BGF, Chapter 1].

Definition B.1. To integers $k_1 \geq 2,\ k_2, \dots, k_d \geq 1$, associate the multiple zeta value

$$\zeta(k_1, \dots, k_d) = \sum_{n_1 > \dots > n_d > 0} \frac{1}{n_1^{k_1} \dots n_d^{k_d}} \in \mathbb{R}.$$

Denote the $\mathbb{Q}$-vector space spanned by all multiple zeta values by

$$\mathcal{Z} = \operatorname{span}_{\mathbb{Q}}\{\zeta(k_1, \dots, k_d) \mid d \geq 0,\ k_1 \geq 2,\ k_2, \dots, k_d \geq 1\},$$

where $\zeta(\emptyset) = 1$. For a multi index $(k_1, \dots, k_d) \in \mathbb{N}^d$, define the weight and depth by

$$\operatorname{wt}(k_1, \dots, k_d) = k_1 + \dots + k_d, \qquad \operatorname{dep}(k_1, \dots, k_d) = d.$$

For simplicity, we will also refer to these numbers as the weight and depth of $\zeta(k_1, \dots, k_d)$.

Numerical experiments have led to the following dimension conjectures for $\mathcal{Z}$.

Conjecture B.2. *([Zag94, p. 509])*
1) The vector space $\mathcal{Z}$ is graded with respect to the weight, i.e.,

$$\mathcal{Z} = \bigoplus_{w \geq 0} \mathcal{Z}^{(w)},$$

where $\mathcal{Z}^{(w)}$ is spanned by the multiple zeta values of weight w.
2) The dimensions of the homogeneous subspaces $\mathcal{Z}^{(w)}$ of $\mathcal{Z}$ are given by

$$H_{\mathcal{Z}}(x) = \sum_{w \geq 0} \dim_{\mathbb{Q}}(\mathcal{Z}^{(w)}) x^w = \frac{1}{1 - x^2 - x^3} = \frac{1}{1 - x^2} \cdot \frac{1}{1 - x^3 - x^5 - x^7 - \dots}.$$

It is well-known that $\mathcal{Z}$ is not graded with respect to the depth, e.g., there is Euler's relation

$$\zeta(2, 1) = \zeta(3).$$

The notion of depth induces an ascending filtration on $\mathcal{Z}$ by

$$\operatorname{Fil}_D^{(d)}(\mathcal{Z}) = \operatorname{span}_{\mathbb{Q}}\{\zeta(k_1, \dots, k_l) \mid \operatorname{dep}(k_1, \dots, k_l) \leq d\}.$$

Considering the associated depth-graded vector space to $\mathcal{Z}$ (as defined in A.48)

$$\operatorname{gr}_D \mathcal{Z} = \bigoplus_{d \geq 0} \operatorname{gr}_D^{(d)} \mathcal{Z} = \bigoplus_{d \geq 0} \operatorname{Fil}_D^{(d)}(\mathcal{Z}) \big/ \operatorname{Fil}_D^{(d-1)}(\mathcal{Z})$$

leads to a refinement of Zagier's dimension conjecture.

Conjecture B.3. *([BK97, (7)]) The dimensions of the homogeneous subspaces of* $\mathrm{gr}_D \mathcal{Z}$ *with respect to the weight and depth are given by*

$$H_{\mathrm{gr}_D \mathcal{Z}}(x,y) = \sum_{w,d\geq 0} \dim_{\mathbb{Q}} \left(\mathrm{gr}_D^{(d)} \mathcal{Z}^{(w)} \right) x^w y^d = (1+E_2(x)y) \frac{1}{1-O_3(x)y+S(x)y^2-S(x)y^4},$$

where

$$E_2(x) = \frac{x^2}{1-x^2}, \qquad O_3(x) = \frac{x^3}{1-x^2}, \qquad S(x) = \frac{x^{12}}{(1-x^4)(1-x^6)}.$$

Proposition B.4. *The space* $\mathcal{Z}$ *equipped with the usual power series multiplication is an algebra.* □

There are two ways of expressing the product of multiple zeta values, called the stuffle and the shuffle product (a general algebraic description is given in Proposition B.20, B.16). The stuffle product comes from the combinatorics of multiplying infinite nested sums. E.g., for $k_1, k_2 \geq 2$, there is the simple calculation

$$\begin{aligned}\zeta(k_1)\zeta(k_2) &= \left(\sum_{m>0} \frac{1}{m^{k_1}} \right) \left(\sum_{n>0} \frac{1}{n^{k_2}} \right) = \left(\sum_{m>n>0} + \sum_{n>m>0} + \sum_{m=n>0} \right) \frac{1}{m^{k_1} n^{k_2}} \\ &= \zeta(k_1,k_2) + \zeta(k_2,k_1) + \zeta(k_1+k_2).\end{aligned}$$

The shuffle product is obtained from expressing multiple zeta values as iterated integrals ([BGF, Theorem 1.108.]). E.g., in depth 2 the shuffle product reads for $k_1, k_2 \geq 2$

$$\zeta(k_1)\zeta(k_2) = \sum_{j=2}^{k_1+k_2-1} \left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1} \right) \zeta(j, k_1+k_2-j).$$

Comparing the stuffle and shuffle product gives the double shuffle relations of multiple zeta values. An immediate consequence of [IKZ06, Proposition 1], is the following.

Proposition B.5. *For all* $k_1, \ldots, k_d \geq 1$*, there are unique elements* $\zeta_{ш}^T(k_1, \ldots, k_d)$ *and* $\zeta_*^T(k_1, \ldots, k_d)$ *in* $\mathcal{Z}[T]$*, such that*

(i) $\zeta_{ш}^T(k_1, \ldots, k_d) = \zeta_*^T(k_1, \ldots, k_d) = \zeta(k_1, \ldots, k_d)$ *for* $k_1 > 1$*,*

(ii) $\zeta_{ш}^T(1) = \zeta_*^T(1) = T$*,*

(iii) all elements $\zeta_{ш}^T(k_1, \ldots, k_d)$ *satisfy the shuffle product formula,*

(iv) all elements $\zeta_*^T(k_1, \ldots, k_d)$ *satisfy the stuffle product formula.* □

Define the $\mathcal{Z}$-linear map $\rho : \mathcal{Z}[T] \to \mathcal{Z}[T]$ by

$$\rho\left(\frac{T^m}{m!} \right) = \sum_{i=0}^{m} \gamma_i \frac{T^{m-i}}{(m-i)!}, \qquad m = 0, 1, 2, \ldots, \tag{B.5.1}$$

where the coefficients $\gamma_i \in \mathcal{Z}$ are defined by $\sum_{i\geq 0} \gamma_i u^i = \exp\left(\sum_{n\geq 2} \frac{(-1)^n}{n} \zeta(n) u^n \right)$.

Theorem B.6. *([IKZ06, Theorem 1]) For all* $k_1, \ldots, k_d \geq 1$*, one has*

$$\rho(\zeta_*^T(k_1, \ldots, k_d)) = \zeta_{ш}^T(k_1, \ldots, k_d).$$

□

From the dimension conjectures B.2 and B.3, one also obtains conjectural dimensions for the algebra $\mathcal{Z}[T]$ spanned by the regularized elements $\zeta_{ш}^T(k_1,\dots,k_d)$ and $\zeta_*^T(k_1,\dots,k_d)$.

Proposition B.7. *Assume that Conjecture B.2 and B.3 hold. Then the Hilbert-Poincare series of $\mathcal{Z}[T]$ and the associated depth-graded space $\mathrm{gr}_D\,\mathcal{Z}[T]$ are given by*

$$\begin{aligned} H_{\mathcal{Z}[T]}(x) &= \frac{1}{1-x}\frac{1}{1-x^2-x^3} = \frac{1}{1-x^2}\frac{1}{1-O_1(x)+E_4(x)}, \\ H_{\mathrm{gr}_D\,\mathcal{Z}[T]}(x,y) &= \frac{1}{1-xy}(1+E_2(x)y)\frac{1}{1-O_3(x)y+S(x)y^2-S(x)y^4} \\ &= (1+E_2(x)y)\frac{1}{1-O_1(x)y+M(x)y^2-xS(x)y^3-S(x)y^4+xS(x)y^5}, \end{aligned}$$

where

$$O_1(x)=\frac{x}{1-x^2}, \qquad E_4(x)=\frac{x^4}{1-x^2}, \qquad M(x)=\frac{1}{(1-x^4)(1-x^6)}. \qquad \square$$

Definition B.8. For $k_1,\dots,k_d\geq 1$, the elements

$$\zeta_{ш}(k_1,\dots,k_d)=\zeta_{ш}^{T=0}(k_1,\dots,k_d), \quad \zeta_*(k_1,\dots,k_d)=\zeta_*^{T=0}(k_1,\dots,k_d) \quad \in \mathcal{Z}$$

are called the shuffle regularized and stuffle regularized multiple zeta values.

Combining the shuffle product formula for the shuffle regularized multiple zeta values and the stuffle product formula for the stuffle regularized multiple zeta values together with Theorem B.6 gives the extended double shuffle relations among multiple zeta values.

Conjecture B.9. *([IKZ06, Conjecture 1]) All algebraic relations in the algebra $\mathcal{Z}$ of multiple zeta values are a consequence of the extended double shuffle relations.*

In particular, Conjecture B.9 would imply that the algebra $\mathcal{Z}$ is graded by weight, since the stuffle and the shuffle product are both homogeneous for the weight.

To get a better understanding of the algebraic structure of $\mathcal{Z}$, it is usual to study the space of indecomposables. More precisely, we want to consider the space of indecomposables of $\mathcal{Z}/\zeta(2)\mathcal{Z}$ given by

$$\mathfrak{nz} = \mathcal{Z}_{\geq 1}\Big/\left(\mathcal{Z}_{\geq 1}^2+\mathbb{Q}\zeta(2)\right). \tag{B.9.1}$$

Here $\mathcal{Z}_{\geq 1}$ denotes the subspace of $\mathcal{Z}$ spanned by all multiple zeta values except $\zeta(\emptyset)=1$. The space $\mathfrak{nz}$ inherits the conjectural weight-grading and the depth filtration from the algebra $\mathcal{Z}$. If $\mathcal{Z}/\zeta(2)\mathcal{Z}$ would be a Hopf algebra, then space of indecomposables $\mathfrak{nz}$ would be equipped with a Lie cobracket (cf. Proposition A.42). It is expected that Goncharov's coproduct defined for formal iterated integrals ([Gon05]) induces a Hopf algebra structure on $\mathcal{Z}/\zeta(2)\mathcal{Z}$, this leads to the following conjectures (according to Theorem A.39, A.43).

Conjecture B.10. *(i) The algebra $\mathcal{Z}$ is a free weight-graded polynomial algebra, more precisely there is an algebra isomorphism*

$$\mathcal{Z}\simeq\mathbb{Q}[\zeta(2)]\otimes\mathcal{U}(\mathfrak{nz}^\vee)^\vee.$$

(ii) The associated depth-graded algebra $\mathrm{gr}_D\,\mathcal{Z}/\zeta(2)\mathcal{Z}$ is a free bi-graded polynomial algebra, it is isomorphic to the graded dual of the universal enveloping algebra of $\mathrm{gr}_D\,\mathfrak{nz}^\vee$.

Some evidence for this conjecture is given by the shape of the conjectured Hilbert-Poincare series in B.2 and B.3.

Lemma B.11. *([IKZ06, Appendix]) By applying Möbius inversion one obtains integers* $g_w,\ g_{w,d} \geq 0$*, such that*

$$H_{\mathcal{Z}/\zeta(2)\mathcal{Z}}(x) \stackrel{?}{=} \frac{1}{1-x^3-x^5-x^7-\dots} = \prod_{w\geq 1}(1-x^i)^{-g_w},$$

$$H_{\mathrm{gr}_D\,\mathcal{Z}/\zeta(2)\mathcal{Z}}(x,y) \stackrel{?}{=} \frac{1}{1-O_3(x)y+S(x)y^2-S(x)y^4} = \prod_{w,d\geq 1}(1-x^w y^d)^{-g_{w,d}}.$$

□

So according to Corollary A.36, the Hilbert-Poincare series of $\mathcal{Z}/\zeta(2)\mathcal{Z}$ resp. $\mathrm{gr}_D\,\mathcal{Z}/\zeta(2)\mathcal{Z}$ could correspond to a universal enveloping algebra of some graded resp. bi-graded Lie algebra. Proposition A.7 implies

Proposition B.12. *(i) If Conjecture B.2 and B.10 (i) hold, then one has for the homogeneous subspaces of weight* $w \geq 1$

$$\dim_{\mathbb{Q}}\left(\mathfrak{nz}^{(w)}\right) = g_w.$$

(ii) If Conjecture B.3 and B.10 (ii) hold, then one has for the homogeneous subspaces of weight $w \geq 1$ *and depth* $d \geq 1$ *that*

$$\dim_{\mathbb{Q}}\left(\mathrm{gr}_D^{(d)}\,\mathfrak{nz}^{(w)}\right) = g_{w,d}.$$

In the following subsections, we will introduce two different explicit Lie algebras, one of them is defined in terms of non-commutative polynomials, the other one uses the language of moulds (Appendix C). For both Lie algebras, it is expected that they are isomorphic to $\mathfrak{nz}^\vee$ equipped with the conjectural Lie bracket induced by Goncharov's coproduct.

B.2 Racinet's Lie algebra of non-commutative polynomials

We provide a summary of the approach of G. Racinet to multiple zeta values given in [Rac00]. We will start with a general description of the stuffle and the shuffle product (p. 189) in terms of quasi-shuffle products (cf Appendix A.3). This allows defining the algebra of formal multiple zeta values $\mathcal{Z}^f$, whose generators satisfy exactly the relations predicted for multiple zeta values in Conjecture B.9. Since quasi-shuffle algebras are always equipped with a Hopf algebra structure (Theorem A.59), one obtains completed dual stuffle and shuffle Hopf algebras (Theorem A.61). The grouplike elements in these completed dual Hopf algebras will give rise to a pro-unipotent affine group scheme DM_0 represented by the algebra $\mathcal{Z}^f$ of formal multiple zeta values modulo $\zeta^f(2)$. By considering the primitive elements in these dual Hopf algebras, one obtains the corresponding Lie algebra functor $\mathfrak{dm}_0$ (cf. Example A.96). This Lie algebra of primitive elements is canonically isomorphic to the graded dual of the Lie coalgebra of indecomposables of $\mathcal{Z}^f$ modulo $\zeta^f(2)$ (cf. Theorem A.43). Note that the group multiplication of the affine group scheme DM_0 equips the algebra $\mathcal{Z}^f/\zeta^f(2)\mathcal{Z}^f$ with a coproduct, which gives rise to the Lie cobracket on the space of indecomposables.

Definition B.13. Let $\mathcal{X} = \{x_0, x_1\}$ be an alphabet. Denote by $\mathcal{X}^*$ the set of all words with letters in $\mathcal{X}$, let $\mathbb{Q}\langle\mathcal{X}\rangle$ be the free algebra generated by $\mathcal{X}$, and denote by $\mathbf{1}$ the empty word. For a word in $\mathbb{Q}\langle\mathcal{X}\rangle$, define the weight and depth as

$$\begin{aligned} \mathrm{wt}(x_0^{k_1-1}x_1 \dots x_0^{k_d-1}x_1x_0^{k_{d+1}}) &= k_1 + \dots + k_{d+1}, \\ \mathrm{dep}(x_0^{k_1-1}x_1 \dots x_0^{k_d-1}x_1x_0^{k_{d+1}}) &= d. \end{aligned}$$

Moreover, the shuffle product $\sqcup\!\sqcup$ on $\mathbb{Q}\langle\mathcal{X}\rangle$ is defined to be the quasi-shuffle product corresponding to $x_i \diamond x_j = 0$ for $i, j \in \{0, 1\}$ (Example A.53 1)), this means one has $\mathbf{1} \sqcup\!\sqcup w = w \sqcup\!\sqcup \mathbf{1} = w$ and

$$x_i u \sqcup\!\sqcup x_j v = x_i(u \sqcup\!\sqcup x_j v) + x_j(x_i u \sqcup\!\sqcup v)$$

for all $u, v, w \in \mathbb{Q}\langle\mathcal{X}\rangle$, $x_i, x_j \in \mathcal{X}$.

Theorem A.59 implies the following.

Proposition B.14. *The tuple* $(\mathbb{Q}\langle\mathcal{X}\rangle, \sqcup\!\sqcup, \Delta_{\mathrm{dec}})$ *is a weight-graded commutative Hopf algebra.*

The deconcatenation coproduct Δ_{dec} is defined in (A.58.1).

For each commutative $\mathbb{Q}$-algebra R with unit, denote by $R\langle\langle\mathcal{X}\rangle\rangle$ the completion of the space $R\langle\mathcal{X}\rangle = \mathbb{Q}\langle\mathcal{X}\rangle \otimes R$ with respect to the weight (Proposition A.45). So $R\langle\langle\mathcal{X}\rangle\rangle$ consists of formal non-commutative power series in the letters x_0, x_1 with coefficients in R. By Theorem A.61 a completed dual to the shuffle Hopf algebra is given by the following.

Proposition B.15. *The tuple* $(R\langle\langle\mathcal{X}\rangle\rangle, \mathrm{conc}, \Delta_{\sqcup\!\sqcup})$ *is a complete cocommutative Hopf algebra, where the coproduct* $\Delta_{\sqcup\!\sqcup}$ *is on the generators defined by*

$$\Delta_{\sqcup\!\sqcup}(x_i) = x_i \otimes \mathbf{1} + \mathbf{1} \otimes x_i, \quad i = 0, 1.$$

The pairing $R\langle\langle\mathcal{X}\rangle\rangle \otimes \mathbb{Q}\langle\mathcal{X}\rangle \to R,\ \phi \otimes w \mapsto (\phi \mid w)$ *gives the duality between the graded Hopf algebra* $(\mathbb{Q}\langle\mathcal{X}\rangle, \sqcup\!\sqcup, \Delta_{\mathrm{dec}})$ *and the complete Hopf algebra* $(R\langle\langle\mathcal{X}\rangle\rangle, \mathrm{conc}, \Delta_{\sqcup\!\sqcup})$.

Let $\mathfrak{h}^1$ be the subspace of $\mathbb{Q}\langle\mathcal{X}\rangle$ spanned by all words ending in x_1, so

$$\mathfrak{h}^1 = \mathbb{Q}\mathbf{1} + \mathbb{Q}\langle\mathcal{X}\rangle x_1.$$

The shuffle product preserves the subspace $\mathfrak{h}^1$, so $(\mathfrak{h}^1, ш)$ is an algebra.

Proposition B.16. *The map*

$$\zeta_{ш} : (\mathfrak{h}^1, ш) \to (\mathcal{Z}, \cdot),$$
$$x_0^{k_1-1}x_1 \dots x_0^{k_d-1}x_1 \mapsto \zeta_{ш}(k_1, \dots, k_d)$$

is a surjective algebra morphism compatible with notions of weight and depth. □

Using the same techniques as in Proposition B.5, one obtains a unique extension of the previously defined map $\mathfrak{h}^1 \to \mathcal{Z}$ to $\mathbb{Q}\langle\mathcal{X}\rangle$. By abuse of notation, we write $\zeta_{ш}(w)$ for the image of $w \in \mathbb{Q}\langle\mathcal{X}\rangle$ under this map.

The duality of $\mathbb{Q}\langle\mathcal{X}\rangle$ and $R\langle\langle\mathcal{X}\rangle\rangle$ given in Proposition B.15 and Proposition B.16 implies that the non-commutative generating series $\phi_{ш} = \sum_{w\in X^*} \zeta_{ш}(w)w \in \mathcal{Z}\langle\langle\mathcal{X}\rangle\rangle$ satisfies

$$\Delta_{ш}(\phi_{ш}) = \phi_{ш}\hat{\otimes}\phi_{ш}. \tag{B.16.1}$$

Next, we introduce the stuffle algebra and equip it with a Hopf algebra structure.

Definition B.17. Consider the infinite alphabet $\mathcal{Y} = \{y_1, y_2, \dots\}$. Let $\mathcal{Y}^*$ be the set of all words with letters in $\mathcal{Y}$, $\mathbb{Q}\langle\mathcal{Y}\rangle$ be the free non-commutative algebra generated by $\mathcal{Y}$, and denote by $\mathbf{1}$ the empty word. For a word in $\mathbb{Q}\langle\mathcal{Y}\rangle$, define the weight and depth by

$$\mathrm{wt}(y_{k_1} \dots y_{k_d}) = k_1 + \dots + k_d, \qquad \mathrm{dep}(y_{k_1} \dots y_{k_d}) = d.$$

Moreover, let the stuffle product $*$ on $\mathbb{Q}\langle\mathcal{Y}\rangle$ be the quasi-shuffle product corresponding to $y_i \diamond y_j = y_{i+j}$ for $i, j \geq 1$, so we have $\mathbf{1} * w = w * \mathbf{1} = w$ and

$$y_i u * y_j v = y_i(u * y_j v) + y_j(y_i u * v) + y_{i+j}(u * v)$$

for all $u, v, w \in \mathbb{Q}\langle\mathcal{Y}\rangle$, $y_i, y_j \in \mathcal{Y}$.

Again one obtains from Theorem A.59.

Proposition B.18. *The tuple $(\mathbb{Q}\langle\mathcal{Y}\rangle, *, \Delta_{\mathrm{dec}})$ is a weight-graded commutative Hopf algebra.*

For any commutative $\mathbb{Q}$-algebra R with unit, denote by $R\langle\langle\mathcal{Y}\rangle\rangle$ the completion of the space $R\langle\mathcal{Y}\rangle = \mathbb{Q}\langle\mathcal{Y}\rangle \otimes R$ with respect to the weight (Definition A.44). Then by Theorem A.61, a completed dual for the stuffle Hopf algebra is given by the following.

Proposition B.19. *The tuple $(R\langle\langle\mathcal{Y}\rangle\rangle, \mathrm{conc}, \Delta_*)$ is a complete cocommutative Hopf algebra, where the coproduct Δ_* is defined on the generators by*

$$\Delta_*(y_i) = \mathbf{1} \otimes y_i + y_i \otimes \mathbf{1} + \sum_{j=1}^{i-1} y_j \otimes y_{i-j}, \quad i = 1, 2, \dots.$$

The pairing $R\langle\langle\mathcal{Y}\rangle\rangle \times \mathbb{Q}\langle\mathcal{Y}\rangle \to R$, $\phi \mid w \mapsto (\phi \mid w)$ gives the duality of $(\mathbb{Q}\langle\mathcal{Y}\rangle, *, \Delta_{\mathrm{dec}})$ and $(R\langle\langle\mathcal{Y}\rangle\rangle, \mathrm{conc}, \Delta_*)$.

Proposition B.20. *The map*

$$\zeta_* : (\mathbb{Q}\langle \mathcal{Y}\rangle, *) \to (\mathcal{Z}, \cdot),$$
$$y_{k_1} \dots y_{k_d} \mapsto \zeta_*(k_1, \dots, k_d)$$

is a surjective algebra morphism compatible with the notions of weight and depth. □

We will write $\zeta_*(w)$ for the image of $w \in \mathbb{Q}\langle \mathcal{Y}\rangle$ under the above map. Proposition B.20 and the duality given in Proposition B.19 imply that the non-commutative generating series $\phi_* = \sum_{w\in\mathcal{Y}^*} \zeta_*(w)w \in \mathcal{Z}\langle\langle \mathcal{Y}\rangle\rangle$ satisfies

$$\Delta_*(\phi_*) = \phi_* \hat{\otimes} \phi_*. \tag{B.20.1}$$

A non-commutative analog of the comparison of the shuffle and stuffle regularized multiple zeta values (Theorem B.6) is given by the following.

Theorem B.21. *([Rac00, III, Corollary 4.20]) The following holds*

$$\phi_* = \exp\left(-\sum_{n\geq 2} \frac{(-1)^n}{n} \zeta(n) y_1^n \right) \Pi_{\mathcal{Y}}(\phi_{ш}),$$

where $\Pi_{\mathcal{Y}}$ *is the* $\mathcal{Z}$*-linear extension of the canonical projection* $\mathbb{Q}\langle \mathcal{X}\rangle \to \mathbb{Q}\langle \mathcal{Y}\rangle$ *sending each word ending in* x_0 *to* 0 *and* $x_1^{k_1-1}x_1 \dots x_0^{k_d-1}x_1$ *to* $y_{k_1} \dots y_{k_d}$ *for all* $k_1, \dots, k_d \geq 1$. □

We reformulated the extended double shuffle relations for multiple zeta values in terms of quasi-shuffle algebras (Proposition B.16, B.20 and Theorem B.21), this leads to the following definition.

Definition B.22. Define the algebra $\mathcal{Z}^f$ of formal multiple zeta values as

$$\mathcal{Z}^f = {(\mathbb{Q}\langle \mathcal{X}\rangle, ш)}\big/{\mathrm{Rel}_{\mathrm{EDS}}},$$

where $\mathrm{Rel}_{\mathrm{EDS}}$ is the ideal generated by the extended double shuffle relations.

In particular, $\mathcal{Z}^f$ is a (weight-)graded algebra generated by the formal symbols $\zeta^f(w)$, $w \in \mathcal{X}^*$, for which we require that they satisfy no other relations than the extended double shuffle relations. Let $\mathfrak{h}^0$ be the subspace of $\mathbb{Q}\langle \mathcal{X}\rangle$ spanned by all words, which start in x_0 and end in x_1, so

$$\mathfrak{h}^0 = \mathbb{Q}\mathbf{1} + x_0 \mathbb{Q}\langle \mathcal{X}\rangle x_1.$$

Using the same techniques as in Proposition B.5, one shows that the elements $\zeta^f(w)$ for words $w \in \mathfrak{h}^0$ generate the space $\mathcal{Z}^f$. Since it is expected that all relations in $\mathcal{Z}$ are a consequence of the extended double shuffle relations (Conjecture B.9), we should have

Conjecture B.23. *The canonical map*

$$\mathcal{Z}^f \to \mathcal{Z},$$
$$\zeta^f(w) \mapsto \zeta(w), \qquad (w \in \mathfrak{h}^0)$$

is an isomorphism of weight-graded algebras.

Definition B.24. For any commutative $\mathbb{Q}$-algebra R with unit, let $\mathsf{DM}(R)$ be the set of all non-commutative power series $\phi \in R\langle\langle \mathcal{X}\rangle\rangle$ satisfying

$$\begin{array}{llll} \text{(i)} & (\phi|x_0) = (\phi|x_1) & = & 0, \\ \text{(ii)} & \Delta_{ш}(\phi) & = & \phi\hat{\otimes}\phi, \\ \text{(iii)} & \Delta_*(\phi_*) & = & \phi_*\hat{\otimes}\phi_*, \end{array}$$

where

$$\phi_* = \exp\left(-\sum_{n\geq 2}\frac{(-1)^n}{n}(\Pi_{\mathcal{Y}}(\phi)|y_n)y_1^n\right)\Pi_{\mathcal{Y}}(\phi) \in R\langle\langle\mathcal{Y}\rangle\rangle$$

and $\Pi_{\mathcal{Y}}$ is the R-linear extension of the projection $\mathbb{Q}\langle\mathcal{X}\rangle \to \mathbb{Q}\langle\mathcal{Y}\rangle$ (cf Theorem B.21).

For each $\lambda \in R$, denote by $\mathsf{DM}_\lambda(R)$ the set of all $\phi \in \mathsf{DM}(R)$, which additionally satisfy

$$\text{(iv)} \qquad (\phi|x_0x_1) = \lambda.$$

By (B.16.1), (B.20.1), and Theorem B.21, the non-commutative generating series $\phi_{ш}$ of the shuffle regularized multiple zeta values is an element in $\mathsf{DM}_{\pi^2/6}(\mathcal{Z})$.

Theorem B.25. *([Rac02, Theorem I]) For each commutative $\mathbb{Q}$-algebra R and $\lambda \in R$, the set $\mathsf{DM}_\lambda(R)$ is non-empty.* □

From [Dr91] and [Fu11] one deduces that there also exist elements ϕ in $\mathsf{DM}_\lambda(R)$ additionally satisfying

$$(\phi \mid x_0^k x_1) = 0 \quad \text{for } k \geq 1 \text{ even.} \tag{B.25.1}$$

The sets $\mathsf{DM}_\lambda(R)$ give rise to an affine scheme represented by a quotient algebra of $\mathcal{Z}^f$ (Appendix A.6).

Proposition B.26. *The functor $\mathsf{DM}_\lambda : \mathbb{Q}\text{-Alg} \to \text{Sets}$ is an affine scheme represented by the algebra $\mathcal{Z}^f / (\zeta^f(2)-\lambda)\mathcal{Z}^f$. In particular, for each commutative $\mathbb{Q}$-algebra R with unit, there is a bijection*

$$\begin{aligned} \mathrm{Hom}_{\mathbb{Q}\text{-Alg}}\left(\mathcal{Z}^f / (\zeta^f(2)-\lambda)\mathcal{Z}^f, R\right) &\to \mathsf{DM}_\lambda(R), \\ \varphi &\mapsto \sum_{w\in\mathcal{X}^*}\varphi(\zeta^f(w))w. \end{aligned}$$

□

To figure out the group structure for the affine scheme DM_0, one needs to consider first the corresponding linearized space.

Definition B.27. For any commutative $\mathbb{Q}$-algebra R with unit, let $\mathfrak{dm}(R)$ be the $\mathbb{Q}$-vector space of all non-commutative polynomials $\psi \in R\langle\mathcal{X}\rangle$ satisfying

$$\begin{array}{llll} \text{(i)} & (\psi \mid x_0) = (\psi \mid x_1) & = & 0, \\ \text{(ii)} & \Delta_{ш}(\psi) & = & \mathbf{1}\otimes\psi + \psi\otimes\mathbf{1}, \\ \text{(iii)} & \Delta_*(\psi_*) & = & \mathbf{1}\otimes\psi_* + \psi_*\otimes\mathbf{1}, \end{array}$$

where

$$\psi_* = \Pi_{\mathcal{Y}}(\psi) + \sum_{n\geq 2}\frac{(-1)^{n-1}}{n}(\Pi_{\mathcal{Y}}(\psi) \mid y_n)y_1^n \in R\langle\mathcal{Y}\rangle$$

and $\Pi_{\mathcal{Y}}$ is the R-linear extension of the canonical projection $\mathbb{Q}\langle\mathcal{X}\rangle \to \mathbb{Q}\langle\mathcal{Y}\rangle$.

By $\mathfrak{dm}_0(R)$ denote the subspace of all $\psi \in \mathfrak{dm}(R)$ additionally satisfying

$$\text{(iv)} \qquad (\psi \mid x_0x_1) = 0.$$

Denote $\mathfrak{dm}_0 = \mathfrak{dm}_0(\mathbb{Q})$. Then one has $\mathfrak{dm}_0(R) = \mathfrak{dm}_0 \otimes R$.

Example B.28. There are the following elements in $\mathfrak{dm}_0$ up to weight 5

$$\begin{aligned}
\xi(3) &= [x_0,[x_0,x_1]] + [[x_0,x_1],x_1],\\
\xi(5) &= [x_0,[x_0,[x_0,[x_0,x_1]]]] + 2[[x_0,[x_0,[x_0,x_1]]],x_1] + \frac{1}{2}[[x_0,[x_0,x_1]],[x_0,x_1]]\\
&\quad + 2[x_1,[x_1,[x_0,[x_0,x_1]]]] - \frac{3}{2}[[x_0,x_1],[[x_0,x_1],x_1]] + [[[[x_0,x_1],x_1],x_1],x_1].
\end{aligned}$$

Proposition B.29. *([Rac00, IV, Proposition 2.2]) For each $k \geq 2$ even and $\psi \in \mathfrak{dm}_0$, one has*

$$(\psi \mid x_0^{k-1}x_1) = 0. \qquad \square$$

Consider the twisted Magnus Lie algebra $(\mathfrak{mt}, \{-,-\})$ given in Theorem 3.7, where $\{-,-\}$ is the Ihara bracket defined by

$$\{\psi_1,\psi_2\} = d_{\psi_1}(\psi_2) - d_{\psi_2}(\psi_1) + [\psi_1,\psi_2], \qquad \psi_1,\psi_2 \in \mathfrak{dm}_0(R),$$

and d_ψ is the derivation given by $d_\psi(\mathbf{1}) = 0$, $d_\psi(x_0) = 0$ and $d_\psi(x_1) = [x_1,\psi]$.

Theorem B.30. *([Rac00, IV, Proposition 2.28., Corollary 3.13.])*
1) The pair $(\mathfrak{dm}_0(R), \{-,-\})$ is a weight-graded Lie subalgebra of the twisted Magnus Lie algebra.

2) Let R be a commutative $\mathbb{Q}$-algebra with unit. For all $\phi_1,\phi_2 \in \mathsf{DM}_\lambda(R)$, there exists a unique element ψ in the completed Lie algebra $\widehat{\mathfrak{dm}_0}(R)$ such that

$$\exp(s_\psi)(\phi_1) = \phi_2,$$

where $s_\psi(f) = d_\psi(f) + f\psi$ for all $f \in R\langle\langle\mathcal{X}\rangle\rangle$. $\square$

In particular, one obtains natural bijections

$$\begin{aligned}
\widehat{\mathfrak{dm}_0}(R) &\to \mathsf{DM}_0(R),\\
\psi &\mapsto \exp(s_\psi)(\mathbf{1}).
\end{aligned} \tag{B.30.1}$$

According to Theorem A.95, this leads to the following.

Corollary B.31. *([Rac00]) The functor DM_0 is a pro-unipotent affine group scheme with Lie algebra functor*

$$\widehat{\mathfrak{dm}_0} : \mathbb{Q}\text{-Alg} \to \text{Lie-Alg}, \;\; R \mapsto \widehat{\mathfrak{dm}_0}(R). \qquad \square$$

Actually, DM_0 is a subscheme of the twisted Magnus affine group scheme MT (Theorem 3.5). So for any commutative $\mathbb{Q}$-algebra R with unit, the group multiplication on $\mathsf{DM}_0(R)$ is given by (Definition 3.3)

$$\phi_1 \circledast \phi_2 = \phi_1\kappa_{\phi_1}(\phi_2), \qquad \phi_1,\phi_2 \in \mathsf{DM}_0(R), \tag{B.31.1}$$

where κ_ϕ is the algebra automorphism on $(R\langle\langle\mathcal{X}\rangle\rangle, \cdot)$ given by $\kappa_\phi(\mathbf{1}) = \mathbf{1}$, $\kappa_\phi(x_0) = x_0$ and $\kappa_\phi(x_1) = \phi^{-1}x_1\phi$.

By [Rac00, Section IV, Corollary 3.13] we have an isomorphism of affine schemes

$$\mathbb{A}^1 \times \widehat{\mathfrak{dm}_0} \to \mathsf{DM}, \tag{B.31.2}$$

where $\mathbb{A}^1$ is the affine scheme from Example A.87 for $V = \mathbb{Q}$. Since the affine scheme DM is represented by the algebra $\mathcal{Z}^f$ (Proposition B.26) and the affine scheme $\widehat{\mathfrak{dm}_0}$ is represented by $\mathcal{S}(\mathfrak{dm}_0^\vee) \simeq \mathcal{U}(\mathfrak{dm}_0)^\vee$ (Proposition A.90, A.35), applying Yoneda's Lemma (Theorem A.81) to (B.31.2) gives the following theorem of Ecalle.

Corollary B.32. *([Rac00], Chapter IV, Corollary 3.14) There is an algebra isomorphism*

$$\mathcal{Z}^f \simeq \mathbb{Q}[\zeta^f(2)] \otimes_{\mathbb{Q}} \mathcal{U}(\mathfrak{dm}_0)^\vee,$$

So, $\mathcal{Z}^f$ is a free polynomial algebra. □

In particular, the conjectured algebra isomorphism $\mathcal{Z}^f \simeq \mathcal{Z}$ (Conjecture B.23) would imply that $\mathcal{Z}$ is a free polynomial algebra (Conjecture B.10).

We want to investigate the dimensions of the homogeneous subspaces of $\mathfrak{dm}_0$. Let $\mathfrak{g}^{\mathfrak{m}} = \mathrm{Lie}\langle s_3, s_5, \ldots\rangle$ be the free Lie algebra generated by formal symbols $s_{2k+1},\ k \geq 1$. From the theory of motivic multiple zeta values ([Bro12],[De89],[Dr91],[Fu11],[Gon05]) it is known that there is a non-canonical injective map

$$\begin{aligned} \mathfrak{g}^{\mathfrak{m}} &\hookrightarrow \mathfrak{dm}_0, \\ s_{2k+1} &\mapsto \sigma_{2k+1}, \end{aligned} \tag{B.32.1}$$

such that $\sigma_{2k+1} \in \mathfrak{dm}_0$ is a homogeneous element of weight $2k+1$. The images σ_{2k+1} are not unique and it is an open question how to explicitly construct them. It is expected that the embedding $\mathfrak{g}^{\mathfrak{m}} \hookrightarrow \mathfrak{dm}_0$ is an isomorphism, this conjecture is attributed to P. Deligne ([De89]) and Y. Ihara ([Ih89, p. 300]).

Conjecture B.33. *The space $\mathfrak{dm}_0$ is a free Lie algebra with exactly one generator in each odd weight $w \geq 3$.*

Under the assumption of Conjecture B.33, one obtains the following Hilbert-Poincare series for the universal enveloping algebra of $\mathfrak{dm}_0$ (Proposition A.8)

$$H_{\mathcal{U}(\mathfrak{dm}_0)}(x) = \sum_{w\geq 0} \dim_{\mathbb{Q}} \left(\mathcal{U}(\mathfrak{dm}_0)^{(w)}\right) x^w = \frac{1}{1 - x^3 - x^5 - x^7 - \ldots}. \tag{B.33.1}$$

Since $\mathcal{U}(\mathfrak{dm}_0)^\vee \simeq \mathcal{Z}^f/_{\zeta(2)\mathcal{Z}^f}$ (Corollary B.32), (B.33.1) would imply that the formal multiple zeta values satisfy Zagier's dimension conjecture B.2. Since it is expected that there is an algebra isomorphism $\mathcal{Z}^f \simeq \mathcal{Z}$ (Conjecture B.23), this gives some evidence for Zagier's dimension conjecture for multiple zeta values.

The group multiplication $\circledast$ on DM_0 given in (B.31.1) induces a Hopf algebra structure on $\mathcal{Z}^f/_{\zeta^f(2)\mathcal{Z}^f}$, since any group multiplication on an affine scheme equips the representing algebra with a Hopf algebra structure (Theorem A.83, Proposition B.26). More precisely, there is a coproduct Δ defined on the non-commutative algebra $\mathbb{Q}\langle\mathcal{X}\rangle$ satisfying

$$(f \circledast g \mid w) = (f \otimes g \mid \Delta(w)) \in R, \qquad f, g \in R\langle\langle\mathcal{X}\rangle\rangle,\ w \in \mathbb{Q}\langle\mathcal{X}\rangle.$$

Here $(\cdot \mid \cdot) : R\langle\langle\mathcal{X}\rangle\rangle \times \mathbb{Q}\langle\mathcal{X}\rangle \to R$ is the canonical pairing given in Proposition B.15. In [BGF, Proposition 3.296] it is shown that this coproduct Δ is exactly Goncharov's coproduct ([Gon05, eq (24)]), hence we denote $\Delta = \Delta^{\mathrm{Gon}}$. The proof is purely algebraic and does not use any motivic results. The coproduct Δ^{Gon} induces a coproduct on $\mathcal{Z}^f/_{\zeta^f(2)\mathcal{Z}^f}$ via the canonical projection

$$\mathbb{Q}\langle\mathcal{X}\rangle \to \mathcal{Z}^f/_{\zeta^f(2)\mathcal{Z}^f},\ w \mapsto \zeta^f(w) \mod \zeta^f(2),$$

for more details see also [Sc13, p.54].

Theorem B.34. *The algebra* $\mathcal{Z}^f/\zeta^f(2)\mathcal{Z}^f$ *equipped with Goncharov's coproduct* Δ^{Gon} *is a Hopf algebra.* □

In particular, by Proposition A.42, Goncharov's coproduct Δ^{Gon} induces a Lie cobracket δ on the space of indecomposables of $\mathcal{Z}^f/\zeta^f(2)\mathcal{Z}^f$ given by

$$\mathfrak{nfz} = \mathcal{Z}^f_{\geq 1}\Big/\Big((\mathcal{Z}^f_{\geq 1})^2 + \mathbb{Q}\zeta^f(2)\Big).$$

Theorem A.89 then implies the following.

Theorem B.35. *There is a canonical isomorphism of Lie algebras*

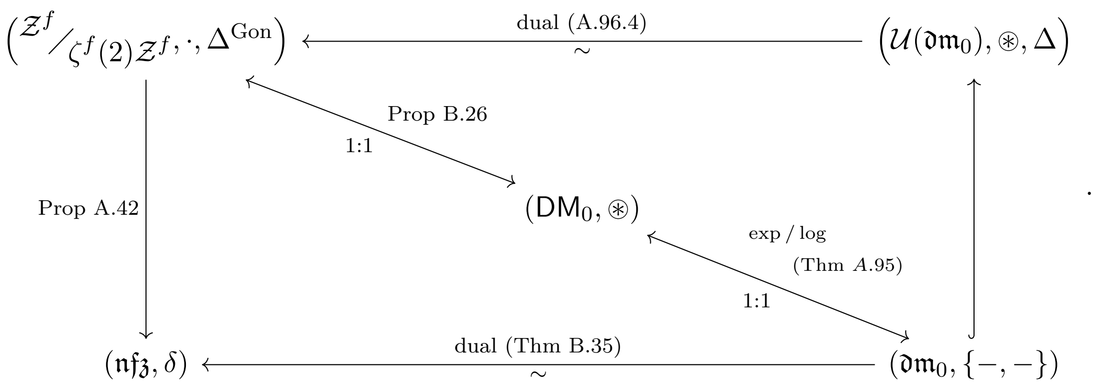
$$\mathfrak{dm}_0 \simeq \mathfrak{nfz}^\vee.$$

Conjecture B.23 would imply that there is an isomorphism $\mathfrak{nz} \simeq \mathfrak{nfz}$, where $\mathfrak{nz}$ is the space of indecomposables of multiple zeta values (see (B.9.1)). In particular under the assumption of Conjecture B.23, one obtains from Corollary B.32 the decomposition

$$\mathcal{Z} \simeq \mathbb{Q}[\zeta(2)] \otimes \mathcal{U}(\mathfrak{nz}^\vee)^\vee$$

as expected in Conjecture B.10 (i).

Summarizing the previous results leads to the following diagram (cf (A.96.3))



(B.35.1)

At the end of this subsection, we want to study the associated depth-graded Lie algebra to $\mathfrak{dm}_0$.

Definition B.36. Define $\mathfrak{ls}$ to be the $\mathbb{Q}$-vector space of all non-commutative polynomials $\psi \in \mathbb{Q}\langle\mathcal{X}\rangle$ satisfying

$$\begin{array}{lcll}
\text{(i)} & (\psi|x_0) = (\psi|x_1) & = & 0, \\
\text{(ii)} & \Delta_{ш}(\psi) & = & \mathbf{1}\otimes\psi + \psi\otimes\mathbf{1}, \\
\text{(iii)} & \Delta_{ш,\mathcal{Y}}(\Pi_{\mathcal{Y}}(\psi)) & = & \mathbf{1}\otimes\Pi_Y(\psi) + \Pi_{\mathcal{Y}}(\psi)\otimes\mathbf{1}, \\
\text{(iv)} & (\psi|x_0^{n-1}x_1) & = & 0 \qquad n \geq 2 \text{ even},
\end{array}$$

where $\Delta_{ш,\mathcal{Y}}$ denotes the shuffle coproduct on $\mathbb{Q}\langle\mathcal{Y}\rangle$ (Example A.62), i.e.,

$$\Delta_{ш,\mathcal{Y}}(y_i) = \mathbf{1}\otimes y_i + y_i \otimes \mathbf{1}, \quad i = 1, 2, \dots ,$$

and $\Pi_{\mathcal{Y}} : \mathbb{Q}\langle\mathcal{X}\rangle \to \mathbb{Q}\langle\mathcal{Y}\rangle$ is the canonical projection given in Theorem B.21.

The same arguments as in the proof of Theorem B.30 1) show

Theorem B.37. *The pair* $(\mathfrak{ls}, \{-,-\})$ *is a bi-graded Lie algebra.* □

Remark B.38. In [Ma22] it is shown that the Lie algebra $(\mathfrak{ls}, \{-,-\})$ is the bi-graded dual of Goncharov's dihedral Lie coalgebra.

Example B.39. For each odd $k \geq 3$, there are the following elements

$$\mathrm{gr}_D\, \xi(k) = \mathrm{ad}(x_0)^{k-1}(x_1) \in \mathfrak{ls}.$$

For example, this implies

$$\begin{aligned}\{\,\mathrm{gr}_D\, \xi(3), \mathrm{gr}_D\, \xi(5)\} = \; & -2[[x_0,[x_0,[x_0,[x_0,[x_0,x_1]]]]],[x_0,x_1]] \\ & -5[[x_0,[x_0,[x_0,[x_0,x_1]]]],[x_0,[x_0,x_1]]] \\ & \in \mathfrak{ls}.\end{aligned}$$

Since $\Delta_{\sqcup\!\sqcup,\mathcal{Y}}$ is the associated depth-graded map to the coproduct Δ_* and by Proposition B.29, one obtains a canonical embedding

$$\mathrm{gr}_D\, \mathfrak{dm}_0 \hookrightarrow \mathfrak{ls}.$$

It is expected that this embedding is an isomorphism. So according to Conjecture B.10 (ii) and Proposition B.12 (ii), the Hilbert-Poincare series of the universal enveloping algebra of $\mathfrak{ls}$ should be given by

$$H_{\mathcal{U}(\mathfrak{ls})}(x,y) = \sum_{w,d\geq 0} \dim_{\mathbb{Q}}(\mathcal{U}(\mathfrak{ls})^{(w,d)})x^w y^d \overset{?}{=} \frac{1}{1-O_3(x)y+S(x)y^2-S(x)y^4}.$$

The dimension formula indicates that the elements σ_{2k+1}, $k \geq 1$, defined in B.32.1 satisfy some relations in $\mathfrak{ls}$. Indeed for any normalized choice of the embedding $\mathfrak{g}^{\mathfrak{m}} \hookrightarrow \mathfrak{dm}_0$, one obtains

$$\sigma_{2k+1} \equiv \mathrm{ad}(x_0)^{2k}(x_1) \;\; \in \;\; \mathfrak{ls},$$

so for example in weight 12 there is the relation

$$\{\sigma_3, \sigma_9\} - 3\{\sigma_5, \sigma_7\} \equiv 0. \tag{B.39.1}$$

Remark B.40. It is expected that $\mathfrak{ls}$ is generated by two Lie algebras $\mathfrak{E}$ and $\mathfrak{C}$, where $\mathfrak{E}$ is generated by the elements $\mathrm{ad}(x_0)^{2k}(x_1)$ and $\mathfrak{C}$ is generated by some elements in depth 4. The generators of the Lie algebra $\mathfrak{E}$ satisfy some relations in depth 2 related to cusp forms (like (B.39.1)) and $\mathfrak{C}$ should be a free Lie algebra. Moreover, there should be no relations between the Lie algebras $\mathfrak{E}$ and $\mathfrak{C}$. This determines the Lie algebra $\mathfrak{ls}$ completely. More details are elaborated in the commutative approach (Subsection B.3).

B.3 Ecalle's commutative approach to Lie algebras via moulds

We will introduce the usual generating series of shuffle and stuffle regularized multiple zeta values and view them as moulds. An introduction to moulds is given in Appendix C, we will use the notations and definitions from there. We will see that the images of the generating series of the shuffle and stuffle regularized multiple zeta values in a formal weight-graded version $\mathcal{T}$ of the space of indecomposables $\mathfrak{nz}$ (see (B.9.1)) are contained in the Lie algebra $\mathrm{ARI}^{\mathrm{pow},\mathcal{T}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$. It is expected that the Lie subalgebra $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ consisting of moulds, whose entries are rational polynomials, is isomorphic to $\mathfrak{nz}^\vee$. Moreover, we will consider also a weight- and depth-graded version of $\mathfrak{nz}$, which leads to a bi-graded Lie algebra $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$. The Lie algebra $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ should be seen as the associated depth-graded Lie algebra to $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$. We will end this section by explaining the structure of the Lie algebra $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ in detail and relating this to the Broadhurst-Kreimer dimension conjecture B.3.

Definition B.41. For any depth $d \geq 1$, define the generating series of the shuffle regularized and stuffle regularized multiple zeta values

$$\begin{aligned} F_d^{⧢}(X_1,\dots,X_d) &= \sum_{k_1,\dots,k_d\geq 1} \zeta_{⧢}(k_1,\dots,k_d) X_1^{k_1-1}\dots X_d^{k_d-1}, \\ F_d^{*}(X_1,\dots,X_d) &= \sum_{k_1,\dots,k_d\geq 1} \zeta_{*}(k_1,\dots,k_d) X_1^{k_1-1}\dots X_d^{k_d-1}. \end{aligned}$$

Moreover, let $F_0^{⧢} = F_0^* = 1$. Then both sequences $F^{⧢} = \left(F_d^{⧢}\right)_{d\geq 0}$ and $F^* = \left(F_d^*\right)_{d\geq 0}$ are moulds in $\mathrm{GARI}^{\mathrm{pow},\mathcal{Z}}$.

For any mould F we denote

$$F^{\#_X}(X_1,\dots,X_d) = F(X_1+\dots+X_d, X_2+\dots+X_d,\dots,X_d).$$

Proposition B.42. *The mould* $\left(F^{⧢}\right)^{\#_X}$ *is symmetral and the mould* F^* *is symmetril.*

Proof. The mould F^* is symmetril, since by Proposition B.20 the coefficient map

$$(\mathbb{Q}\langle\mathcal{Y}\rangle,*) \to (\mathcal{Z},\cdot),\ y_{k_1}\dots y_{k_d} \mapsto \zeta_*(k_1,\dots,k_d)$$

is an algebra morphism (cf Example A.72). Moreover,

$$(\mathfrak{h}^1,⧢) \to (\mathcal{Z},\cdot),\ x_0^{k_1-1}x_1\dots x_0^{k_d-1}x_1 \mapsto \zeta_{⧢}(k_1,\dots,k_d)$$

is an algebra morphism (Proposition B.16), so we deduce from (A.69.1) that for all $0 < n < d$

$$\begin{aligned} &\left(F^{⧢}\right)^{\#_X}(X_1,\dots,X_n)\left(F^{⧢}\right)^{\#_X}(X_{n+1},\dots,X_d) \\ &\qquad = \zeta_{⧢}\circ\iota_{\mathcal{Y}}\Big(\rho_{\mathcal{Y}}(\mathcal{W})(X_1,\dots,X_n) ⧢ \rho_{\mathcal{Y}}(\mathcal{W})(X_{n+1},\dots,X_d)\Big)^{\#_X}. \end{aligned}$$

Since by definition $\zeta_{⧢}\circ\iota_{\mathcal{Y}}\Big(\rho_{\mathcal{Y}}(\mathcal{W})(X_1,\dots,X_d)\Big) = F^{⧢}(X_1,\dots,X_d)$ for all $d \geq 1$, the mould $\left(F^{⧢}\right)^{\#_X}$ is symmetral (cf Example A.72). □

Definition B.43. Let $\mathcal{I} = \bigoplus_{w\geq 1} \mathcal{Z}^{(w)}$, where $\mathcal{Z}^{(w)}$ denotes the homogeneous subspace of $\mathcal{Z}$ of weight w. Define the $\mathbb{Q}$-algebra

$$\mathcal{T} = {}^{\mathcal{I}}\big/_{\left(\mathcal{I}^2 + \mathbb{Q}\zeta(2)\right)}.$$

By construction, the algebra $\mathcal{T}$ is graded by weight and all products of multiple zeta values become trivial in $\mathcal{T}$. In particular, the dimension of $\mathcal{T}^{(w)}$ equals the number of algebra generators of $\mathcal{Z}/_{\zeta(2)\mathcal{Z}}$ in weight w. If the algebra $\mathcal{Z}$ would be graded (Conjecture B.2), then $\mathcal{T}$ is equal to the space of indecomposables $\mathfrak{nz}$ (see (B.9.1)).

Denote by $\overline{\zeta_{ш}}(k_1, \ldots, k_d)$ the images of the shuffle regularized multiple zeta values in $\mathcal{T}$, by $\overline{\zeta_*}(k_1, \ldots, k_d)$ the images of the stuffle regularized multiple zeta values in $\mathcal{T}$, and consider their generating series in some depth $d \geq 1$,

$$\overline{F_d^{ш}}(X_1, \ldots, X_d) = \sum_{k_1,\ldots,k_d \geq 1} \overline{\zeta_{ш}}(k_1, \ldots, k_d) X_1^{k_1-1} \ldots X_d^{k_d-1},$$
$$\overline{F_d^{*}}(X_1, \ldots, X_d) = \sum_{k_1,\ldots,k_d \geq 1} \overline{\zeta_{*}}(k_1, \ldots, k_d) X_1^{k_1-1} \ldots X_d^{k_d-1}.$$

Set $\overline{F_0^{ш}} = \overline{F_0^{*}} = 0$, then both sequences $\overline{F^{ш}} = \left(\overline{F_d^{ш}}\right)_{d\geq 0}$ and $\overline{F^{*}} = \left(\overline{F_d^{*}}\right)_{d\geq 0}$ are moulds contained in $\mathrm{ARI}^{\mathrm{pow},\mathcal{T}}$.

Corollary B.44. *The mould* $\left(\overline{F^{ш}}\right)^{\#x}$ *is alternal and the mould* $\overline{F^{*}}$ *is alternil.*

Proof. This is an immediate consequence of Proposition B.42, since alternality (resp. alternility) is just symmetrality (resp. symmetrility) modulo products (see Appendix C.1). □

There is an explicit relation between the shuffle and the stuffle regularized multiple zeta values given in Theorem B.6, which allows treating $\left(\overline{F^{ш}}\right)^{\#x}$ and $\overline{F^{*}}$ simultaneously.

Theorem B.45. *The mould* $\left((-1)^{d-1}(\overline{F_d^{ш}})^{\#x}\right)_{d\geq 0}$ *is contained in*

$$\mathrm{ARI}^{\mathrm{pow},\mathcal{T}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}} = \left\{ A \in \mathrm{ARI}^{\mathrm{pow},\mathcal{T}} \;\middle|\; \begin{array}{l} \cdot\ A \textit{ is alternal,} \\ \cdot\ \mathrm{swap}(A) \textit{ is alternil up to addition with some} \\ \quad \textit{constant mould,} \\ \cdot\ A_1(X_1) \textit{ is even.} \end{array} \right\}.$$

Proof. By Corollary B.44, the mould $(\overline{F^{ш}})^{\#x}$ is alternal, and therefore also the mould $\left((-1)^{d-1}(\overline{F_d^{ш}})^{\#x}\right)_{d\geq 0}$ is alternal. By definition of the map ρ (given in (B.5.1)) and Theorem B.6, the images of $\zeta_{ш}(k_1, \ldots, k_d)$ and $\zeta_*(k_1, \ldots, k_d)$ in $\mathcal{T}$ become equal up to addition with some constant,

$$\overline{F_d^{ш}}(X_1, \ldots, X_d) = \overline{F_d^{*}}(X_1, \ldots, X_d) + C_d$$

for some $C_d \in \mathcal{T}$. Moreover, any alternal mould A satisfies

$$\mathrm{swap}(A)(X_1, \ldots, X_d) = (-1)^{d-1} A^{\#\overset{-1}{x}}(X_1, \ldots, X_d), \qquad d \geq 1.$$

So Corollary B.44 implies that there is a constant mould $(C_d)_{d\geq 0}$, such that

$$\mathrm{swap}\left((-1)^{d-1}(\overline{F_d^{ш}})^{\#x}\right)_{d\geq 0} + (C_d)_{d\geq 0} = (\overline{F_d^{ш}})_{d\geq 0} + (C_d)_{d\geq 0} = (\overline{F_d^{*}})_{d\geq 0}$$

is an alternil mould. Finally, Euler's formula for the even single zeta values

$$\zeta(2k) \in \mathbb{Q}\pi^k, \quad k \geq 1,$$

implies that the odd component of $\left(\overline{F_1^{ш}}\right)^{\#x} = \overline{F_1^{ш}}$ vanishes. □

Lemma B.46. *Decompose the mould $\overline{F^{ш}}$ of the shuffle regularized multiple zeta values as*

$$\overline{F^{ш}} = \sum_{\alpha} \alpha \cdot \xi^{\alpha},$$

where α runs through a vector space basis of $\mathcal{T}$. Then every mould $\left((-1)^{d-1}(\xi^{\alpha})^{\#_X}\right)_{d\geq 0}$ is contained in

$$\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}} = \left\{ A \in \mathrm{ARI}^{\mathrm{pow},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}} \;\middle|\; \begin{array}{l} \cdot\ A_d(X_1,\dots,X_d) \in \mathbb{Q}[X_1,\dots,X_d] \textit{ for all } d\geq 1, \\ \cdot\ A_d(X_1,\dots,X_d) \neq 0 \textit{ only for finitely many } d \geq 1 \end{array} \right\}.$$

Proof. Since the mould $\left((-1)^{d-1}(\overline{F^{ш}_d})^{\#_X}\right)_{d\geq 0}$ is contained in $\mathrm{ARI}^{\mathrm{pow},\mathcal{T}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ (Theorem B.45) and we decompose over a $\mathbb{Q}$-vector space basis of $\mathcal{T}$, the moulds $\left((-1)^{d-1}(\xi^{\alpha})^{\#_X}\right)_{d\geq 0}$ must be contained in $\mathrm{ARI}^{\mathrm{pow},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$. Since $\mathcal{T}$ is graded by weight and the homogeneous components are finite-dimensional, the components of each mould $\left((-1)^{d-1}(\xi^{\alpha})^{\#_X}\right)_{d\geq 0}$ must be polynomial. Moreover, the depth is bounded by the weight, therefore only finitely many components can be non-zero. □

Example B.47. There are the following moulds in $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$, which should correspond to the elements $\overline{\zeta}(3), \overline{\zeta}(5) \in \mathcal{T}$

$$\begin{aligned} \xi(3) &= (X_1^2,\ -X_1+X_2,\ 0,\ \dots) \\ \xi(5) &= (X_1^4,\ -2X_1^3+2X_2^3-\frac{1}{2}X_1^2X_2+\frac{1}{2}X_1X_2^2,\ 2X_1^2-4X_2^2+2X_3^2-\frac{3}{2}X_1X_2+3X_1X_3 \\ &\quad -\frac{3}{2}X_2X_3,\ -X_1+3X_2-3X_3+X_4,\ 0,\ \dots) \end{aligned}$$

The space $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ is graded by weight, its homogeneous components $\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}\right)^{(w)}$ are defined in (C.24.1).

Corollary B.48. *For each $w \geq 1$, the following holds*

$$\dim_{\mathbb{Q}} \mathcal{T}^{(w)} \leq \dim_{\mathbb{Q}} \left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}\right)^{(w)}.$$

Proof. Let α is a basis element of $\mathcal{T}^{(w)}$, then by Lemma B.46 $\left((-1)^{d-1}(\xi^{\alpha})^{\#_X}\right)_{d\geq 0}$ is contained in $\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}\right)^{(w)}$. Therefore, the dimension of the space spanned by the moulds $\left((-1)^{d-1}(\xi^{\alpha})^{\#_X}\right)_{d\geq 0}$, where α is homogeneous of weight w, is bounded by the dimension of $\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}\right)^{(w)}$. Evidently the assignment $\alpha \mapsto \left((-1)^{d-1}(\xi^{\alpha})^{\#_X}\right)_{d\geq 0}$ is injective, thus also the dimension of $\mathcal{T}^{(w)}$ has an upper bound given by $\dim_{\mathbb{Q}} \left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}\right)^{(w)}$. □

Theorem B.49. *([Sc15, Theorem 4.6.1.]) For each commutative $\mathbb{Q}$-algebra R with unit, the space $\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ equipped with the ari bracket (Definition C.22) is a graded Lie algebra.* □

Recall that it is expected that $\mathcal{T} = \mathfrak{nz}$. The decomposition in Lemma B.46 should be seen just as a dualizing process with respect to the weight-grading, thus there should be a Lie algebra isomorphism $\mathfrak{nz}^{\vee} \simeq \mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$. So Conjecture B.10 (i) and Proposition B.12 (i) can be reformulated in terms of bimoulds as follows.

Conjecture B.50. *(i) There is an algebra isomorphism*

$$\mathcal{Z} \simeq \mathbb{Q}[\zeta(2)] \otimes \mathcal{U}\big(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}\big)^{\vee}.$$

(ii) For all $w \geq 1$, the following holds

$$\dim_{\mathbb{Q}} \big(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}\big)^{(w)} = \dim_{\mathbb{Q}} \mathcal{T}^{(w)} = g_w,$$

where the numbers g_w are defined in Lemma B.11.

Next, we want to consider the associated depth-graded space to $\mathcal{T}$ (Definition B.43).

Definition B.51. Define the $\mathbb{Q}$-algebra

$$\mathcal{M} = \bigoplus_{w,d\geq 1} \mathcal{M}^{(w,d)}, \qquad \mathcal{M}^{(w,d)} = \mathrm{gr}_D^{(d)} \mathcal{T}^{(w)} = {}^{\mathrm{Fil}_D^{(d)}(\mathcal{T}^{(w)})}\big/_{\mathrm{Fil}_D^{(d-1)}(\mathcal{T}^{(w)})}.$$

The algebra $\mathcal{M}$ is bi-graded with respect to weight and depth and the product is trivial. In particular, the dimension of the homogeneous space $\mathcal{M}^{(w,d)}$ equals the number of algebra generators of $\mathrm{gr}_D\, {}^{\mathcal{Z}}\!/_{\zeta(2)\mathcal{Z}}$ of weight w and depth d. As before, Conjecture B.2 would imply that $\mathcal{M} = \mathrm{gr}_D\, \mathfrak{nz}$.

Denote by $\mathrm{gr}_D\, \overline{\zeta_{ш}}(k_1, \ldots, k_d)$ the images of the shuffle-regularized multiple zeta values in $\mathcal{M}$ and by $\mathrm{gr}_D\, \overline{\zeta_*}(k_1, \ldots, k_d)$ the images of the stuffle-regularized multiple zeta values in $\mathcal{M}$. For some depth $d \geq 1$ consider their generating series,

$$\begin{aligned}
\mathrm{gr}_D\, \overline{F^{ш}_d}(X_1, \ldots, X_d) &= \sum_{k_1,\ldots,k_d\geq 1} \mathrm{gr}_D\, \overline{\zeta_{ш}}(k_1, \ldots, k_d) X_1^{k_1-1} \ldots X_d^{k_d-1}, \\
\mathrm{gr}_D\, \overline{F^{*}_d}(X_1, \ldots, X_d) &= \sum_{k_1,\ldots,k_d\geq 1} \mathrm{gr}_D\, \overline{\zeta_{*}}(k_1, \ldots, k_d) X_1^{k_1-1} \ldots X_d^{k_d-1}.
\end{aligned}$$

Set $\mathrm{gr}_D\, \overline{F^{ш}_0} = \mathrm{gr}_D\, \overline{F^{*}_0} = 0$, then $\mathrm{gr}_D\, \overline{F^{ш}} = \big(\mathrm{gr}_D\, \overline{F^{ш}_d}\big)_{d\geq 0}$ and $\mathrm{gr}_D\, \overline{F^{*}} = \big(\mathrm{gr}_D\, \overline{F^{*}_d}\big)_{d\geq 0}$ are moulds in $\mathrm{ARI}^{\mathrm{pow},\mathcal{M}}$.

Proposition B.52. *Both $\big(\mathrm{gr}_D\, \overline{F^{ш}}\big)^{\#_X}$ and $\mathrm{gr}_D\, \overline{F^{*}}$ are alternal moulds. In addition, one has*

$$\mathrm{gr}_D\, \overline{F^{ш}} = \mathrm{gr}_D\, \overline{F^{*}}.$$

Proof. The first part is a direct consequence of Corollary B.44 and the observation that alternility modulo lower depth is just alternality. The second part is obtained from Theorem B.6 and the definition of ρ (given in (B.5.1)). □

Theorem B.53. *The mould $\big(\mathrm{gr}_D\, \overline{F^{ш}}\big)^{\#_X}$ is contained in*

$$\mathrm{ARI}^{\mathrm{pow},\mathcal{M}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}} = \left\{ A \in \mathrm{ARI}^{\mathrm{pol},\mathcal{M}} \;\middle|\; \begin{array}{l} \cdot\ A \textit{ is alternal}, \\ \cdot\ \mathrm{swap}(A) \textit{ is alternal}, \\ \cdot\ A_1(X_1) \textit{ is even.} \end{array} \right\}.$$

Proof. As explained in the proof of Theorem B.45, one has

$$\mathrm{swap}\Big(\big(\mathrm{gr}_D\, \overline{F^{ш}}\big)^{\#_X}\Big)(X_1, \ldots, X_d) = (-1)^{d-1}\, \mathrm{gr}_D\, \overline{F}^{ш}(X_1, \ldots, X_d).$$

Moreover, observe that for any alternal mould A also the mould $\big((-1)^{d-1}A\big)_{d\geq 0}$ is alternal. So Proposition B.52 implies that $\big(\mathrm{gr}_D\, \overline{F^{ш}}\big)^{\#_X}$ and $\mathrm{swap}\Big(\big(\mathrm{gr}_D\, \overline{F^{ш}}\big)^{\#_X}\Big)$ are both alternal. Finally, Euler's formula $\zeta(2k) \in \mathbb{Q}\pi^k$, $k \geq 1$, implies that $\big(\mathrm{gr}_D\, \overline{F^{ш}_1}\big)^{\#_X}$ is even. □

Lemma B.54. *Decompose* $\mathrm{gr}_D\,\overline{F^{\sqcup\!\sqcup}}$ *over a* $\mathbb{Q}$*-vector space basis of* $\mathcal{M}$*,*

$$\mathrm{gr}_D\,\overline{F^{\sqcup\!\sqcup}} = \sum_\beta \beta \cdot \mathrm{gr}_D\,\xi^\beta.$$

Then any bimould $\left(\mathrm{gr}_D\,\xi^\beta\right)^{\#_X}$ *is contained in*

$$\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}} = \left\{ A \in \mathrm{ARI}^{\mathrm{pow},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}} \;\middle|\; \begin{array}{l} \cdot\ A_d(X_1,\dots,X_d) \in \mathbb{Q}[X_1,\dots,X_d] \text{ for all } d \geq 1, \\ \cdot\ A_d(X_1,\dots,X_d) \neq 0 \text{ only for finitely many } d \geq 1 \end{array} \right\}.$$

Proof. Similar to Lemma B.46, this follows immediately from the weight-grading of $\mathcal{M}$. ☐

For example, the moulds

$$\mathrm{gr}_D\,\xi(k) = \left(X_1^{k-1},\ 0,\ \dots\right), \qquad k \geq 3 \text{ odd},$$

are contained in $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$, and should correspond to the odd zeta values $\mathrm{gr}_D\,\overline{\zeta}(k)$.

The space $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ is bi-graded by weight and depth, the homogeneous components $\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(w,d)}$ are given in (C.24.2).

Corollary B.55. *([IKZ06, Corollary 7]) For each* $w, d \geq 1$*, the following holds*

$$\dim_{\mathbb{Q}} \mathcal{M}^{(w,d)} \leq \dim_{\mathbb{Q}} \left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(w,d)}.$$

Proof. This follows from the same arguments as in Corollary B.48. ☐

Theorem B.56. *([Sc15], Theorem 2.5.6.) For each commutative* $\mathbb{Q}$*-algebra* R *with unit, the space* $\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ *is a bi-graded Lie algebra with the ari bracket (Definition C.22).* ☐

It is expected that $\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ is exactly the associated depth-graded Lie algebra to $\mathrm{ARI}^{\mathrm{pol},R}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$. So as a reformulation of Conjecture B.10 (ii) and Proposition B.12 (ii), the following should hold.

Conjecture B.57. *(i) There is an algebra isomorphism*

$$\mathrm{gr}_D\,{}^{\mathcal{Z}}\!/_{\zeta(2)\mathcal{Z}} \simeq \mathcal{U}\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^\vee.$$

(ii)([IKZ06, p. 329]) For all $w, d \geq 1$*, the following holds*

$$\dim_{\mathbb{Q}} \left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(w,d)} = \dim_{\mathbb{Q}} \mathcal{M}^{(w,d)} = g_{w,d},$$

where the numbers $g_{w,d}$ *are obtained in Lemma B.11.*

Computational evidence for the second part of this conjecture are given by Carr and Ecalle in [Ec11, 7.10.].

At the end of this subsection, we will explain the structure of the Lie algebra $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ and relate this to the Broadhurst-Kreimer dimension conjecture B.3. For simplicity we work over the field $\mathbb{Q}$, but the same holds for any commutative $\mathbb{Q}$-algebra R with unit.

Proposition B.58. *([Ec11, eq (2.79)]) If* $w, d \geq 1$ *and* $w \not\equiv d \mod 2$*, then one has*

$$\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(w,d)} = \{0\}.$$

☐

Definition B.59. Let $\mathfrak{E}$ be the Lie subalgebra of $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ spanned by the ekma moulds

$$\mathrm{gr}_D\,\xi(k) = (X_1^{k-1}, 0, \ldots), \qquad k \geq 3 \text{ odd}.$$

Since the depth 1 components of moulds in $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ must be even, we must have

$$\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(1)} = \mathfrak{E}^{(1)}.$$

To describe the relations between the ekma moulds we introduce the space of even period polynomials (see [KZ84] for details). For $k \geq 2$ even, set

$$W_k^{\mathrm{ev}} = \left\{ f \in \mathbb{Q}[x,y] \;\middle|\; \begin{array}{l} \cdot\ f \text{ homogeneous of degree } k-2, \\ \cdot\ f(x,y) + f(y,x) = 0, \\ \cdot\ f(\pm x, \pm y) = f(x,y), \\ \cdot\ f(x,y) + f(x-y,x) + f(-y,x-y) = 0. \end{array} \right\}.$$

There is a decomposition

$$W_k^{\mathrm{ev}} = \mathbf{S}_k \oplus \mathbb{Q}p_{k-2},$$

where $p_{k-2} \in W_k^{\mathrm{ev}}$ denotes the polynomial $p_{k-2} = x^{k-2} - y^{k-2}$. By the Eichler-Shimura theorem, there is an isomorphism

$$\mathcal{S}_k^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z})) \to \mathbf{S}_k,$$

here $\mathcal{S}_k^{\mathbb{Q}}(\mathrm{SL}_2(\mathbb{Z}))$ denotes the space of cusp forms with rational coefficients for $\mathrm{SL}_2(\mathbb{Z})$.

Proposition B.60. *([Bro21, 7.2.]) There is a short exact sequence*

$$0 \to \bigoplus_{k \geq 2 \text{ even}} \mathbf{S}_k \to \left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(1)} \wedge \left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(1)} \xrightarrow{\mathrm{ari}} \left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(2)} \to 0.$$

□

In particular, one has $\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(2)} = \mathfrak{E}^{(2)}$, and each relation in depth 2 between the ekma moulds $\mathrm{gr}_D\,\xi(k)$, $k \geq 3$ odd, can be uniquely assigned to a cusp form. One can also show that $\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(3)} = \mathfrak{E}^{(3)}$ and all relations in depth 3 are induced from the cusp form relations in depth 2 ([Bro21, 7.3]).

In depth 4, one obtains a proper inclusion $\mathfrak{E}^{(4)} \subsetneq \left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(4)}$. We will explain now how to obtain the additional generators in $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ of depth 4, this construction is due to Ecalle ([Ec11, Section 7.3, 7.7]).
Consider the relation in $\mathfrak{E}^{(2)}$ corresponding to the smallest cusp form in weight 12,

$$\mathrm{ari}\Big(\mathrm{gr}_D\,\xi(3), \mathrm{gr}_D\,\xi(9)\Big) - 3\,\mathrm{ari}\Big(\mathrm{gr}_D\,\xi(5), \mathrm{gr}_D\,\xi(7)\Big) = 0.$$

Lifting this relation to the non depth-graded space $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$, one obtains

$$\mathrm{ari}\Big(\xi(3), \xi(9)\Big) - 3\,\mathrm{ari}\Big(\xi(5), \xi(7)\Big) = \xi_\Delta$$

where $\xi_\Delta \in \mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ is a mould of depth ≥ 4. Since it is expected that $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$ is the associated depth-graded Lie algebra to $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$, any relation between the ekma moulds in depth 2 should have a lift to $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$. By construction, this lift vanishes in depth 2 and due to Proposition B.58 also the depth 3 part vanishes. So any relation between the ekma moulds in depth 2 should yield an element in $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}$ and after taking the depth-graded part a (possibly trivial) in $\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(4)}$.

Definition B.61. Let $\mathfrak{C}$ be the Lie algebra generated by the elements in $\left(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}\right)^{(4)}$ induced by the relations in $\mathfrak{E}^{(2)}$ in the above explained way.

In [Bro21, 8.2] a different construction for the generators of $\mathfrak{C}$ is given.

Definition B.62. Any even period polynomial $f \in \bigoplus_{k\geq 2 \text{ even}} \mathbf{S}_k$ has a decomposition

$$f(x,y) = xyf_1(x,y) = xy(x-y)f_0(x,y)$$

for some homogeneous $f_1, f_0 \in \mathbb{Q}[x,y]$. Define the polynomial

$$\mathbf{e}_f(z_0,z_1,z_2,z_3,z_4) = \sum_{\mathbb{Z}/5\mathbb{Z}} f_1(z_4-z_3, z_2-z_1) + (z_0-z_1)f_0(z_2-z_3, z_4-z_3),$$

where the sum is taken over all cyclic permutations of z_0, z_1, z_2, z_3, z_4. Then the mould $\mathrm{carma}_f \in \mathrm{ARI}$ is given by

$$\mathrm{carma}_f(X_1,X_2,X_3,X_4) = \mathbf{e}_f(0, X_1, X_1+X_2, X_1+X_2+X_3, X_1+X_2+X_3+X_4)$$

and 0 elsewhere.

Proposition B.63. *([Bro21, Theorem 8.2]) For each $f \in \bigoplus_{k\geq 2 \text{ even}} \mathbf{S}_k$, the mould* carma_f *is contained in* $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$. □

The following structure is expected for the two Lie subalgebras $\mathfrak{E}$ and $\mathfrak{C}$.

Conjecture B.64. *([Bro21, Conjecture 3], [Ec11, 8.5.])*

(i) There are no relations between the two Lie subalgebras $\mathfrak{E}$ and $\mathfrak{C}$ and both together generate the Lie algebra $\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}$.

(ii) The Lie algebra $\mathfrak{C}$ is a free Lie algebra generated by the moulds carma_f *(Definition B.62).*

(iii) The only relations in the Lie algebra $\mathfrak{E}$ are the cusp form relations in depth 2 *(Proposition B.60).*

Assuming Conjecture B.64, one obtains the following Hilbert-Poincare series (cf (A.11.1))

$$\begin{aligned} H_{\mathcal{U}(\mathfrak{E})}(x,y) &= \sum_{w,d\geq 0} \dim_{\mathbb{Q}} \left(\mathcal{U}(\mathfrak{E})^{(w,d)}\right) x^w y^d &&= \tfrac{1}{1-O_3(x)y+S(x)y^2}, \\ H_{\mathcal{U}(\mathfrak{C})}(x,y) &= \sum_{w,d\geq 0} \dim_{\mathbb{Q}} \left(\mathcal{U}(\mathfrak{C})^{(w,d)}\right) x^w y^d &&= \tfrac{1}{1-S(x)y^4}, \\ H_{\mathcal{U}(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}})}(x,y) &= \sum_{w,d\geq 0} \dim_{\mathbb{Q}} \left(\mathcal{U}(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}})^{(w,d)}\right) x^w y^d &&= \tfrac{1}{1-O_3(x)y+S(x)y^2-S(x)y^4}, \end{aligned}$$

where

$$O_3(x) = \frac{x^3}{1-x^2}, \qquad S(x) = \sum_{k\geq 12} \dim \mathcal{S}_k(\mathrm{SL}_2(\mathbb{Z}))x^k = \frac{x^{12}}{(1-x^4)(1-x^6)}.$$

In particular, the Hilbert-Poincare series of $\mathcal{U}(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}})$ equals the conjectured Hilbert-Poincare series of $\mathrm{gr}_D\, \mathcal{Z}/\zeta(2)\mathcal{Z}$ in the Broadhurst-Kreimer conjecture B.3. This gives some evidence for the expected isomorphy $\mathrm{gr}_D\, \mathcal{Z}/\zeta(2)\mathcal{Z} \simeq \mathcal{U}(\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}})^{\vee}$ (Conjecture B.57 (i)).

B.4 Comparison of the different approaches

In the previous two subsections, we have seen two different Lie algebras conjecturally isomorphic to the dual of the space of indecomposables $\mathfrak{nz}$ (see (B.9.1)), one is defined in the context of non-commutative polynomials (B.2) and the other one is defined via moulds (B.3). We will give an explicit isomorphism between these two Lie algebras, a proof is given in [Rac00, Appendix A] or [Sc15, Chapter 3]. The relation of these two kinds of generating series is generally explained in Subsection A.4.

Definition B.65. For each $k \geq 1$, define

$$C_k = \mathrm{ad}(x_0)^{k-1}(x_1)$$

and let $\mathcal{C}$ be the alphabet consisting of these letters. For a word in $\mathbb{Q}\langle\mathcal{C}\rangle$, define the weight and depth by

$$\mathrm{wt}(C_{k_1}\dots C_{k_d}) = k_1 + \dots + k_d, \qquad \mathrm{dep}(C_{k_1}\dots C_{k_d}) = d.$$

Proposition B.66. *(Lazard elimination, [Re93, Theorem 0.6]) The space* $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{C}\rangle$ *is a free Lie algebra and*

$$\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{X}\rangle = \mathbb{Q}x_0 \oplus \mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{C}\rangle. \qquad \square$$

In particular, both Lie algebras $\mathfrak{dm}_0$ (Definition B.27) and $\mathfrak{ls}$ (Definition B.36) are contained in $\mathrm{Lie}_{\mathbb{Q}}\langle\mathcal{C}\rangle$.

Definition B.67. Consider the $\mathbb{Q}$-linear map

$$\begin{aligned} \rho_{\mathcal{C}} : \mathbb{Q}\langle\mathcal{C}\rangle &\to \mathbb{Q}[X_1, X_2, \dots], \\ C_{k_1}\dots C_{k_d} &\mapsto X_1^{k_1-1}\dots X_d^{k_d-1}. \end{aligned}$$

To every element $f \in \mathbb{Q}\langle\mathcal{C}\rangle$ associate a mould $\mathrm{ma}(f) = \big(\mathrm{ma}(f)_d\big)_{d\geq 0} \in \mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}$ by

$$\mathrm{ma}(f)_d(X_1, \dots, X_d) = (-1)^{d-1}\rho_{\mathcal{C}}(f^{(d)}),$$

where $f^{(d)}$ denotes the homogeneous component of f of depth d.

Theorem B.68. *([Sc15, Theorem 3.4.3., Theorem 3.4.4.,]) There are two Lie algebra isomorphisms*

$$\begin{aligned} (\mathfrak{dm}_0, \{-,-\}) &\xrightarrow{\sim} (\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}}, \mathrm{ari}), \quad f \mapsto \mathrm{ma}(f) \\ (\mathfrak{ls}, \{-,-\}) &\xrightarrow{\sim} (\mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}}, \mathrm{ari}), \quad f \mapsto \mathrm{ma}(f) \end{aligned} \qquad \square$$

In particular, one obtains the following commutative diagram of Lie algebras

$$\begin{array}{ccc} \mathfrak{dm}_0 & \xrightarrow[\mathrm{ma}]{\sim} & \mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}*\underline{\mathrm{il}}} \\ \downarrow{\scriptstyle \mathrm{gr}_D} & & \downarrow{\scriptstyle \mathrm{gr}_D} \\ \mathfrak{ls} & \xrightarrow[\mathrm{ma}]{\sim} & \mathrm{ARI}^{\mathrm{pol},\mathbb{Q}}_{\underline{\mathrm{al}}/\underline{\mathrm{al}}} \end{array}$$

Example B.69. The elements $\xi(3), \xi(5)$ introduced in Example B.28 can be expressed in terms of the alphabet C as

$$\xi(3) = C_3 + [C_2, C_1],$$
$$\xi(5) = C_5 + 2[C_4, C_1] + \frac{1}{2}[C_3, C_2] + 2[C_1, [C_1, C_3]] - \frac{3}{2}[C_2, [C_2, C_1]] + [[[C_2, C_1], C_1], C_1].$$

Thus, we compute

$$\begin{aligned}
\rho_{\mathcal{C}}\Big(\xi(3)\Big) &= (X_1^2,\ -X_1 + X_2,\ 0,\ \ldots), \\
\rho_{\mathcal{C}}\Big(\xi(5)\Big) &= (X_1^4,\ -2X_1^3 + 2X_2^3 - \frac{1}{2}X_1^2 X_2 + \frac{1}{2}X_1 X_2^2,\ 2X_1^2 - 4X_2^2 + 2X_3^2 \\
&\qquad - \frac{3}{2}X_1 X_2 + 3X_1 X_3 - \frac{3}{2}X_2 X_3,\ -X_1 + 3X_2 - 3X_3 + X_4,\ 0,\ \ldots)
\end{aligned}$$

These two moulds coincide with the ones given in Example B.47.

B.5 Block grading

The generators σ_{2k+1} of the depth-graded Lie algebra $\mathfrak{ls}$ satisfy relations related to modular forms (see for example (B.39.1)). One way to rid of these algebraic dependencies of the generators σ_{2k+1} is to consider the block degree instead of the depth. Following [Ch21], define for a word $w = x_{i_1} \dots x_{i_w}$ in $\mathbb{Q}\langle\mathcal{X}\rangle$ its block degree as

$$\deg_{\mathrm{bl}}(w) = \#\{m \mid i_m = i_{m+1}\}.$$

This defines an decreasing filtration on the space $\mathbb{Q}\langle\mathcal{X}\rangle$

$$\mathrm{Fil}_{\mathrm{bl}}^{(n)} \mathbb{Q}\langle\mathcal{X}\rangle = \mathrm{span}_{\mathbb{Q}}\{w \in \mathcal{X}^* \mid \deg_{\mathrm{bl}}(x_1 w x_0) \geq n\}.$$

Proposition B.70. *The Lie algebra $(\mathfrak{dm}_0, \{-,-\})$ is filtered for the block degree. In particular,*

$$\mathrm{gr}_{\mathrm{bl}}\, \mathfrak{dm}_0 = \bigoplus_{n\geq 0} \mathrm{Fil}_{\mathrm{bl}}^{(n)}\, \mathfrak{dm}_0 \big/ \mathrm{Fil}_{\mathrm{bl}}^{(n+1)}\, \mathfrak{dm}_0$$

is a block-graded Lie algebra equipped with the block-graded Ihara bracket. □

There is an explicit formula for the block-graded Ihara bracket. For $\psi \in \mathbb{Q}\langle\mathcal{X}\rangle$, define the map $d_\psi^{\mathrm{bl}} : \mathbb{Q}\langle\mathcal{X}\rangle \to \mathbb{Q}\langle\mathcal{X}\rangle$ by

$$d_\psi^{\mathrm{bl}}(x_0^m x_1^n) = \begin{cases} 0, & n = 0 \\ x_0^m x_1^n \psi, & m = 0 \\ x_0^m x_1^n \psi + x_0^m \psi^* x_1^n & \text{else} \end{cases}$$

and extend this to

$$d_\psi^{\mathrm{bl}}(x_0^{m_1} x_1^{n_1} \dots x_0^{m_r} x_1^{n_r} x_0^{m_{r+1}}) = \sum_{i=1}^{r} x_0^{m_1} x_1^{n_1} \dots x_0^{m_{i-1}} x_1^{n_{i-1}} d_\psi^{\mathrm{bl}}(x_0^{m_i} x_1^{n_i}) x_0^{m_{i+1}} x_1^{n_{i+1}} \dots x_0^{m_r} x_1^{n_r} x_0^{m_{r+1}}$$

for all $r \geq 1,\ m_2, \dots, m_r, n_1, \dots n_r \geq 1,\ m_1, m_{r+1} \geq 0$. Moreover, let

$$\Pi_{x_1} : \mathbb{Q}\langle\mathcal{X}\rangle \to \mathbb{Q}\mathbf{1} + x_0\mathbb{Q}\langle\mathcal{X}\rangle$$

be the canonical projection, which sends any word starting with x_1 to 0 and is the identity elsewhere. Then the block-graded Ihara bracket is given by

$$\{\psi_1, \psi_2\}^{\mathrm{bl}} = d_{\psi_1}^{\mathrm{bl}}(\psi_2) - d_{\psi_2}^{\mathrm{bl}}(\psi_1) + \psi_1 \Pi_{x_1}(\psi_2) - \psi_2 \Pi_{x_1}(\psi_1).$$

Theorem B.71. *([Ke20, Proposition 2.2.5, Theorem 2.2.7, Proposition 2.3.3])*
1) The image of $\mathfrak{g}^{\mathfrak{m}}$ in $\left(\mathrm{gr}_{\mathrm{bl}}\, \mathfrak{dm}_0, \{-,-\}^{\mathrm{bl}}\right)$ is a free Lie algebra with exactly one generator p_{2k+1} in each odd weight ≥ 3.

2) The generators p_{2k+1} are explicitly determined and for each normalized choice of the embedding $\mathfrak{g}^{\mathfrak{m}} \hookrightarrow \mathfrak{dm}_0$, one has

$$\sigma_{2k+1} \equiv p_{2k+1} \ \in\ \mathrm{gr}_{\mathrm{bl}}\, \mathfrak{dm}_0.$$ □

Corollary B.72. *Assume that $\mathfrak{dm}_0$ is a free Lie algebra with one generator in each odd weight ≥ 3 (Conjecture B.33). Then the pair $(\mathrm{gr}_{\mathrm{bl}}\, \mathfrak{dm}_0, \{-,-\}^{\mathrm{bl}})$ is also a free Lie algebra generated by one element in each odd weight $w \geq 3$. In particular, we would have*

$$\mathrm{gr}_{\mathrm{bl}}\, \mathfrak{dm}_0 \simeq \mathfrak{dm}_0.$$

Appendix C Moulds and bimoulds

This chapter provides the necessary background on moulds and bimoulds. These objects were introduced by J. Ecalle ([Ec11], [Ec02]) and further developed by L. Schneps ([Sc15]). To compare the following to these articles, one needs to identify $X_i = v_i$ and $Y_i = u_i$.

Definition C.1. Let $\mathcal{A}$ be an alphabet, denote by $\mathcal{A}^*$ the set of all words with letters in $\mathcal{A}$, and let R be a commutative $\mathbb{Q}$-algebra with unit. Following [Cr09], a mould is a map

$$\begin{aligned} M : \mathcal{A}^* &\to R, \\ w &\mapsto M(w). \end{aligned}$$

There is a canonical bijection between the sets of moulds $\mathcal{A}^* \to R$ and non-commutative power series over $\mathcal{A}$ with coefficients in R given by the association

$$(M : \mathcal{A}^* \to R) \mapsto \sum_{w \in \mathcal{A}^*} M(w)w. \tag{C.1.1}$$

Example C.2. (i) The map of the balanced multiple q-zeta values given in Theorem 2.59 defines a mould

$$\begin{aligned} M_{\zeta_q} : \mathcal{B}^* &\to \mathcal{Z}_q, \\ b_{s_1} \dots b_{s_l} &\mapsto \begin{cases} \zeta_q(s_1, \dots, s_l) & \text{if } s_1 > 0 \\ 0 & \text{else} \end{cases} \qquad (s_1, \dots, s_l \geq 0). \end{aligned}$$

(ii) Similarly, the map of the shuffle regularized multiple zeta values from Proposition B.16 gives a mould

$$\begin{aligned} M_{\zeta_{ш}} : \mathcal{X}^* &\to \mathcal{Z}, \\ x_0^{k_1-1}x_1 \dots x_0^{k_d-1}x_1x_0^{k_{d+1}-1} &\mapsto \begin{cases} \zeta_{ш}(k_1, \dots, k_d), & k_{d+1} = 1 \\ 0, & \text{else} \end{cases} \qquad (k_1, \dots, k_{d+1} \geq 1). \end{aligned}$$

By choosing an appropriate translation map ρ from the algebra $\mathbb{Q}\langle\mathcal{A}\rangle$ into some ring of commutative polynomials with coefficients in R, one can associate to a mould $M : \mathcal{A}^* \to R$ a sequence of commutative generating series with coefficients in R (cf Subsection A.4, Definition A.70). This leads to the notion of moulds, which will be used in this work.

Example C.3. Consider the $\mathbb{Q}$-linear map

$$\begin{aligned} \rho_{\mathcal{X}} : \mathbb{Q}\langle\mathcal{X}\rangle &\to \mathbb{Q}[X_1, X_2, \dots], \\ x_0^{k_1-1}x_1 \dots x_0^{k_d-1}x_1x_0^{k_{d+1}-1} &\mapsto \begin{cases} X_1^{k_1-1} \dots X_d^{k_d-1}, & k_{d+1} = 1 \\ 0, & \text{else} \end{cases}, \end{aligned}$$

which satisfies the conditions in Definition A.64, and the mould $M_{\zeta_{ш}}$ given in Example C.2 (ii). Then the commutative generating series with coefficients in $\mathcal{Z}$ associated to $(M_{\zeta_{ш}}, \rho_{\mathcal{X}})$ in the sense[9] of Definition A.70 is given by

$$(M_{\zeta_{ш}} \otimes \rho_{\mathcal{X}})(\mathcal{W})_d(X_1, \dots, X_d) = \sum_{w \in (\mathcal{X}^*)^{(d)}} M_{\zeta_{ш}}(w)\rho_{\mathcal{X}}(w), \quad d \geq 1,$$

where $(\mathcal{X}^*)^{(d)}$ denotes the subset of all words in $\mathcal{X}^*$ of depth d. Observe that generating series $(M_{\zeta_{ш}} \otimes \rho_{\mathcal{X}})(\mathcal{W})_d(X_1, \dots, X_d)$ equals exactly the generating series of the shuffle regularized multiple zeta values $F^{ш}(X_1, \dots, X_d)$ in some depth d (Definition B.41).

[9] More precisely, the map $M_{\zeta_{ш}} : \mathcal{X}^* \to \mathcal{Z}$ need to be extended to the space $\mathbb{Q}\langle\mathcal{X}\rangle$ by $\mathbb{Q}$-linearity to apply Definition A.70

In particular, we will view moulds from now on as a sequence of commutative power series in an increasing number of variables.

Definition C.4. Let R be a commutative $\mathbb{Q}$-algebra with unit. A sequence

$$M = (M_d(X_1, \ldots, X_d))_{d\geq 0} = (M_0(\emptyset), M_1(X_1), M_2(X_1, X_2), \ldots) \in \prod_{d\geq 0} R[[X_1, \ldots, X_d]]$$

is called a mould. Denote $\mathrm{MU}^{\mathrm{pow},R} = \prod_{d\geq 0} R[[X_1, \ldots, X_d]]$ and call the elements in $\mathrm{MU}^{\mathrm{pow},R}$ moulds with coefficients in R.

Let $\mathcal{A} = \{a_1, a_2, \ldots\}$ be an alphabet. Conversely, any mould $M \in \mathrm{MU}^{\mathrm{pow},R}$ defines a mould in the sense of Definition C.1

$$\begin{aligned} M : \mathcal{A}^* &\to R[[X_1, X_2, \ldots]], \\ a_{i_1} \ldots a_{i_d} &\mapsto M_d(X_{i_1}, \ldots, X_{i_d}). \end{aligned}$$

In particular, the alphabet $\mathcal{A}$ gets identified with the set of variables $\{X_1, X_2, \ldots\}$.

At some points, it is necessary to consider sequences

$$M = (M_d(X_1, \ldots, X_d))_{d\geq 0} \in \prod_{d\geq 0} R((X_1, \ldots, X_d)).$$

We denote the set of those moulds by $\mathrm{MU}^{\mathrm{fL},R} = \prod_{d\geq 0} R((X_1, \ldots, X_d))$.

Definition C.5. A sequence

$$M = \left(M_d \begin{pmatrix} X_1, \ldots, X_d \\ Y_1, \ldots, Y_d \end{pmatrix} \right)_{d\geq 0} = \left(M_0(\emptyset), M_1 \begin{pmatrix} X_1 \\ Y_1 \end{pmatrix}, M_2 \begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix}, \ldots \right) \in \prod_{d\geq 0} R[[X_1, Y_1, \ldots, X_d, Y_d]]$$

is called a bimould. Denote $\mathrm{BIMU}^{\mathrm{pow},R} = \prod_{d\geq 0} R[[X_1, Y_1, \ldots, X_d, Y_d]]$ and call the elements in $\mathrm{BIMU}^{\mathrm{pow},R}$ bimoulds with coefficients in R.

Consider a bi-alphabet $\mathcal{A}_{\mathrm{bi}} = \{a_{i,j} \mid i, j \geq 1\}$. Then any bimould $M \in \mathrm{BIMU}^{\mathrm{pow},R}$ gives a mould in the sense of Definition C.1

$$\begin{aligned} M : \mathcal{A}_{\mathrm{bi}}^* &\to R[[X_1, Y_1, X_2, Y_2, \ldots]], \\ a_{i_1,j_1} \ldots a_{i_d,j_d} &\mapsto M_d \begin{pmatrix} X_{i_1}, \ldots, X_{i_d} \\ Y_{j_1}, \ldots, Y_{j_d} \end{pmatrix}. \end{aligned}$$

Moreover, set $\mathrm{BIMU}^{\mathrm{fL},R} = \prod_{d\geq 0} R((X_1, Y_1, \ldots, X_d, Y_d))$.

Example C.6. The generating series of the SZ multiple q-zeta values (2.23.1) given by $\mathfrak{sz}_0 = 1$ and for $d \geq 1$ by

$$\mathfrak{sz}_d \begin{pmatrix} X_1, \ldots, X_d \\ Y_1, \ldots, Y_d \end{pmatrix} = \sum_{\substack{k_1,\ldots,k_d\geq 1 \\ m_1,\ldots,m_d\geq 0}} \zeta_q^{\mathrm{SZ}}(k_1, \{0\}^{m_1}, \ldots, k_d, \{0\}^{m_d}) X_1^{k_1-1} Y_1^{m_1} \ldots X_d^{k_d-1} Y_d^{m_d}$$

and the generating series of the bi-brackets (2.32.1) given by $\mathfrak{g}_0 = 1$ and for $d \geq 1$ by

$$\mathfrak{g}_d \begin{pmatrix} X_1, \ldots, X_d \\ Y_1, \ldots, Y_d \end{pmatrix} = \sum_{\substack{k_1,\ldots,k_d\geq 1 \\ m_1,\ldots,m_d\geq 0}} g \begin{pmatrix} k_1, \ldots, k_d \\ m_1, \ldots, m_d \end{pmatrix} X_1^{k_1-1} \frac{Y_1^{m_1}}{m_1!} \ldots X_d^{k_d-1} \frac{Y_d^{m_d}}{m_d!}$$

both define bimoulds $\mathfrak{sz} = (\mathfrak{sz}_d)_{d\geq 0}$ and $\mathfrak{g} = (\mathfrak{g}_d)_{d\geq 0}$ in $\mathrm{BIMU}^{\mathrm{pow},\mathcal{Z}_q}$.

In the following, we will often give definitions only for bimoulds. By forgetting about the second row corresponding to the variables Y_i, one obtains the definition for moulds. Moreover, we will usually omit the index d and simply write $M\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix}$ resp. $M(X_1,\dots,X_d)$. If the shape of the components of the bimoulds does not matter, we just write BIMU^R (resp. MU^R). Similarly, if the underlying algebra R is clear from the context, we just write BIMU (resp. MU). This applies also to all subsets of (bi-)moulds, which will be defined in the following.

Definition C.7. For two bimoulds $M, N \in \mathrm{BIMU}^R$ and $\lambda \in R$, define

$$\begin{aligned}
(\lambda M)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} &= \lambda \cdot M\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix}, \\
(M+N)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} &= M\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} + N\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix}, \\
\mathrm{mu}(M,N)\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} &= \sum_{i=0}^{d} M\begin{pmatrix} X_1,\dots,X_i \\ Y_1,\dots,Y_i \end{pmatrix} N\begin{pmatrix} X_{i+1},\dots,X_d \\ Y_{i+1},\dots,Y_d \end{pmatrix}.
\end{aligned}$$

The composition mu corresponds to the power series multiplication under the bijection (C.1.1).

Lemma C.8. *The triples* $(\mathrm{BIMU}^R, +, \mathrm{mu})$ *and* $(\mathrm{MU}^R, +, \mathrm{mu})$ *are R-algebras with unit.* □

Define the following subspaces of MU and BIMU,

$$\mathrm{ARI} = \{A \in \mathrm{MU} \mid A_0 = 0\}, \qquad \mathrm{BARI} = \{A \in \mathrm{BIMU} \mid A_0 = 0\}.$$

A simple calculation shows the following.

Lemma C.9. *The sets* ARI^R *and* BARI^R *are R-subalgebras of* $(\mathrm{BIMU}^R, +, \mathrm{mu})$.

Moreover, define the subsets

$$\mathrm{GARI} = \{A \in \mathrm{MU} \mid A_0 = 1\}, \qquad \mathrm{GBARI} = \{A \in \mathrm{BIMU} \mid A_0 = 1\}.$$

C.1 Basic symmetries of (bi-)moulds

We will introduce some standard symmetries of (bi-)moulds. All of them are introduced in [Ec11] and can be found with more details in [Sc15]. We focus on giving an as explicit description of these symmetries as possible. All of the following (bi-)moulds will have coefficients in some fixed $\mathbb{Q}$-algebra R with unit.

The first symmetry for bimoulds is closely related to the conjugation of partitions.

Definition C.10. For $A \in \mathrm{BIMU}$, define the bimould swap(A) as

$$\mathrm{swap}(A)\binom{X_1,\ldots,X_d}{Y_1,\ldots,Y_d} = A\binom{Y_1+\cdots+Y_d, Y_1+\cdots+Y_{d-1},\ldots,Y_1}{X_d, X_{d-1}-X_d,\ldots,X_1-X_2}.$$

In this special case, consider on both sides the row consisting of the variables X_i to obtain the corresponding definition for moulds, i.e., for a mould $A \in \mathrm{MU}$, one has

$$\mathrm{swap}(A)(X_1,\ldots,X_d) = A(X_d, X_{d-1}-X_d,\ldots,X_1-X_2).$$

The inverse of swap on MU is obtained by only considering the variables Y_i.

A (bi-)mould A is called swap invariant if swap$(A) = A$.

Example C.11. Let $A \in \mathrm{BIMU}^{\mathrm{pow}}$ and write

$$A\binom{X_1,\ldots,X_d}{Y_1,\ldots,Y_d} = \sum_{\substack{k_1,\ldots,k_d\geq 1\\ m_1,\ldots,m_d\geq 0}} a\binom{k_1,\ldots,k_d}{m_1,\ldots,m_d} X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\cdots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}$$

where $a\binom{k_1,\ldots,k_d}{m_1,\ldots,m_d}$ are the (normalized) coefficients of A. If the bimould A is swap invariant, then the coefficients satisfy

$$a\binom{k_1}{m_1} = \frac{m_1!}{(k_1-1)!}a\binom{m_1+1}{k_1-1},$$
$$a\binom{k_1,k_2}{m_1,m_2} = \sum_{u=0}^{m_1}\sum_{v=0}^{k_2-1}\frac{(-1)^v}{u!v!}\frac{m_1!}{(k_1-1)!}\frac{(m_2+u)!}{(k_2-1-v)!}a\binom{m_2+1+u, m_1+1-u}{k_2-1-v, k_1-1+v}.$$

In higher depths, it is hard to give the explicit relations between the coefficients of A coming from the swap invariance, see for example [BI22, Remark 3.14].

We want to translate the shuffle product and the q-stuffle product defined on $\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle$ (Example A.53, 1) and 5)) into the language of (bi-)moulds (cf Subsection A.4). So recall that $\mathcal{Y}^{\mathrm{bi}} = \{y_{k,m} \mid k \geq 1,\ m \geq 0\}$ and that the depth of a word in $\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle$ is given by $\mathrm{dep}(y_{k_1,m_1}\cdots y_{k_d,m_d}) = d$. Define the $\mathbb{Q}$-linear map

$$\rho_{\mathcal{Y}^{\mathrm{bi}}}: \mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle \to \mathbb{Q}[X_1,Y_1,X_2,Y_2,\ldots],$$
$$y_{k_1,m_1}\cdots y_{k_d,m_d} \mapsto X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\cdots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!},$$

which satisfies the properties in Definition A.64. The generating series of words in $\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle$ associated to $\rho_{\mathcal{Y}^{\mathrm{bi}}}$ is given by $\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_0 = \mathbf{1}$ and

$$\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})_d\binom{X_1,\ldots,X_d}{Y_1,\ldots,Y_d} = \sum_{\substack{k_1,\ldots,k_d\geq 1\\ m_1,\ldots,m_d\geq 0}} y_{k_1,m_1}\cdots y_{k_d,m_d}X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\cdots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!},\quad d\geq 1.$$

Definition C.12. Consider the shuffle algebra $(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, ⧢)$, i.e., $⧢$ is the corresponding quasi-shuffle product to $y_{k_1,m_1} \diamond y_{k_2,m_2} = 0$ (Example A.53, 1)). A bimould $A \in \mathrm{GBARI}^{\mathrm{pow},R}$ is called symmetral if there is an algebra morphism $\varphi_⧢ : (\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, ⧢) \to R$, such that for all $d \geq 1$

$$A_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1 \\ m_1,\dots,m_d\geq 0}} \varphi_⧢(y_{k_1,m_1}\cdots y_{k_d,m_d}) X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\cdots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}.$$

In other words, the bimould A is symmetral if and only if A is $(\varphi_⧢, \rho_{\mathcal{Y}^{\mathrm{bi}}})$-symmetric in the sense of Definition A.71. We will refer to the map $\varphi_⧢$ as the coefficient map of A.

Denote by $\mathrm{GBARI}^{\mathrm{pow},R}_{\mathrm{as}}$ (resp. $\mathrm{GARI}^{\mathrm{pow},R}_{\mathrm{as}}$) the subset of all symmetral bimoulds (resp. moulds).

As obtained in (A.71.1) a bimould $A \in \mathrm{GBARI}^{\mathrm{pow},R}$ is symmetral with coefficient map $\varphi_⧢$ if and only if for all $0 < n < d$

$$A\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} A\begin{pmatrix} X_{n+1},\dots,X_d \\ Y_{n+1},\dots,Y_d \end{pmatrix} = \varphi_⧢\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} ⧢ \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix} X_{n+1},\dots,X_d \\ Y_{n+1},\dots,Y_d \end{pmatrix}\right).$$

An explicit recursive formula for $⧢$ on the generating series of words $\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})$ is obtained in Corollary A.76.

Definition C.13. Let$(\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *)$ be the q-stuffle algebra, i.e., $*$ is the quasi-shuffle product with $y_{k_1,m_1} \diamond y_{k_2,m_2} = y_{k_1+k_2,m_1+m_2}$ (Example A.53, 6)). A bimould $A \in \mathrm{GBARI}^{\mathrm{pow},R}$ is said to be symmetril if there is an algebra morphism $\varphi_* : (\mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle, *) \to R$, such that for all $d \geq 1$

$$A_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1 \\ m_1,\dots,m_d\geq 0}} \varphi_*(y_{k_1,m_1}\cdots y_{k_d,m_d}) X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\cdots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}.$$

In particular, the bimould A is symmetril if and only if A is $(\varphi_*, \rho_{\mathcal{Y}^{\mathrm{bi}}})$-symmetric. As before, we also refer to φ_* as the coefficient map of A.

By $\mathrm{GBARI}^{\mathrm{pow},R}_{\mathrm{is}}$ (resp. $\mathrm{GARI}^{\mathrm{pow},R}_{\mathrm{is}}$) denote the subset of all symmetril bimoulds (resp. moulds).

A bimould $A \in \mathrm{GBARI}^{\mathrm{pow},R}$ is symmetril with coefficient map φ_* if and only if for all $0 < n < d$

$$A\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} A\begin{pmatrix} X_{n+1},\dots,X_d \\ Y_{n+1},\dots,Y_d \end{pmatrix} = \varphi_*\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix} X_1,\dots,X_n \\ Y_1,\dots,Y_n \end{pmatrix} * \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix} X_{n+1},\dots,X_d \\ Y_{n+1},\dots,Y_d \end{pmatrix}\right).$$

An explicit recursive formula for the product $*$ on these generating series of words $\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})$ is given in Corollary A.77.

Example C.14. For a bimould $A \in \mathrm{GBARI}$, symmetrility in depths 2 and 3 means

$$A\begin{pmatrix}X_1\\Y_1\end{pmatrix}\cdot A\begin{pmatrix}X_2\\Y_2\end{pmatrix} = A\begin{pmatrix}X_1,X_2\\Y_1,Y_2\end{pmatrix} + A\begin{pmatrix}X_2,X_1\\Y_2,Y_1\end{pmatrix} + \frac{1}{X_1-X_2}\left(A\begin{pmatrix}X_1\\Y_1+Y_2\end{pmatrix} - A\begin{pmatrix}X_2\\Y_1+Y_2\end{pmatrix}\right),$$

$$\begin{aligned}A\begin{pmatrix}X_1\\Y_1\end{pmatrix}\cdot A\begin{pmatrix}X_2,X_3\\Y_2,Y_3\end{pmatrix} &= A\begin{pmatrix}X_1,X_2,X_3\\Y_1,Y_2,Y_3\end{pmatrix} + A\begin{pmatrix}X_2,X_1,X_3\\Y_2,Y_1,Y_3\end{pmatrix} + A\begin{pmatrix}X_2,X_3,X_1\\Y_2,Y_3,Y_1\end{pmatrix}\\ &\quad + \frac{1}{X_1-X_2}\left(A\begin{pmatrix}X_1,X_3\\Y_1+Y_2,Y_3\end{pmatrix} - A\begin{pmatrix}X_2,X_3\\Y_1+Y_2,Y_3\end{pmatrix}\right)\\ &\quad + \frac{1}{X_1-X_3}\left(A\begin{pmatrix}X_2,X_1\\Y_2,Y_1+Y_3\end{pmatrix} - A\begin{pmatrix}X_2,X_3\\Y_2,Y_1+Y_3\end{pmatrix}\right).\end{aligned}$$

Omit all terms of lower depths to obtain the formulas for symmetrality.

Remark C.15. (i) So far we defined symmetrality and symmetrility only for (bi-)moulds in $\mathrm{GBARI}^{\mathrm{pow},R}$, but clearly one could use the complicated explicit formulas for such symmetries (as given in Example C.14 for low depths) alternatively as the definition for these symmetries. This is for example the point of view of J. Ecalle and L. Schneps ([Ec11],[Sc15]), and in turn this allows to extend these symmetries to a wider class of (bi-) moulds like $\mathrm{GBARI}^{\mathrm{fL},R}$.

(ii) The definition of symmetral and symmetril for moulds is already given in Example A.72, but can be also obtained from Definition C.12 and C.13 by forgetting about the variables Y_i and the second index of the letters in $\mathcal{Y}^{\mathrm{bi}}$.

Consider the subspace

$$\mathrm{BARI}_{\mathrm{is,swap}} = \left\{ A \in \mathrm{BARI} \;\middle|\; \begin{array}{l}\cdot\ A \text{ symmetril,}\\ \cdot\ A \text{ swap invariant}\end{array}\right\}.$$

The elements in $\mathrm{BARI}_{\mathrm{is,swap}}$ satisfy a second product formula. More precisely, one obtains this second formula by applying the swap invariance to both factors, then multiplying with respect to $*$ and finally again applying the swap invariance to all terms. For example in depth 2, this leads to the following explicit formula

$$A\begin{pmatrix}X_1\\Y_1\end{pmatrix} A\begin{pmatrix}X_2\\Y_2\end{pmatrix} = A\begin{pmatrix}X_1+X_2,X_1\\Y_2,Y_1-Y_2\end{pmatrix} + A\begin{pmatrix}X_1+X_2,X_2\\Y_1,Y_2-Y_1\end{pmatrix} + \frac{A\begin{pmatrix}X_1+X_2\\Y_1\end{pmatrix} - A\begin{pmatrix}X_1+X_2\\Y_2\end{pmatrix}}{Y_1-Y_2}. \tag{C.15.1}$$

There are two other important properties of bimoulds, which should be seen as the symmetrality and symmetrility modulo products.

Definition C.16. A bimould $A \in \mathrm{BARI}^{\mathrm{pow},R}$ is called alternal if there is a $\mathbb{Q}$-linear map $\varphi_{\sqcup\!\sqcup} : \mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle \to R$ satisfying $\varphi_{\sqcup\!\sqcup}(u \sqcup\!\sqcup v) = 0$ for all $u,v \in \mathbb{Q}\langle\mathcal{Y}^{\mathrm{bi}}\rangle\backslash\mathbb{Q}\mathbf{1}$, such that for all $d \geq 1$

$$A_d\begin{pmatrix}X_1,\dots,X_d\\Y_1,\dots,Y_d\end{pmatrix} = \sum_{\substack{k_1,\dots,k_d\geq 1\\ m_1,\dots,m_d\geq 0}} \varphi_{\sqcup\!\sqcup}(y_{k_1,m_1}\dots y_{k_d,m_d}) X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\dots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}.$$

In this case, we also call $\varphi_{\sqcup\!\sqcup}$ the coefficient map of A.

Denote by $\mathrm{BARI}_{\mathrm{al}}^{\mathrm{pow},R}$ (resp. $\mathrm{ARI}_{\mathrm{al}}^{\mathrm{pow},R}$) the subspace of all alternal bimoulds (resp. moulds).

In particular, a bimould $A \in \mathrm{BARI}^{\mathrm{pow},R}$ is alternal with coefficient map $\varphi_{\sqcup\!\sqcup}$ if and only if for all $0 < n < d$

$$\varphi_{\sqcup\!\sqcup}\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_1,\ldots,X_n\\Y_1,\ldots,Y_n\end{pmatrix} \sqcup\!\sqcup\, \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+1},\ldots,X_d\\Y_{n+1},\ldots,Y_d\end{pmatrix}\right) = 0. \tag{C.16.1}$$

Definition C.17. A bimould $A \in \mathrm{BARI}^{\mathrm{pow},R}$ is called alternil if there is a $\mathbb{Q}$-linear map $\varphi_* : \mathbb{Q}\langle \mathcal{Y}^{\mathrm{bi}}\rangle \to R$ satisfying $\varphi_*(u * v) = 0$ for all $u, v \in \mathbb{Q}\langle \mathcal{Y}^{\mathrm{bi}}\rangle \backslash \mathbb{Q}\mathbf{1}$, such that for all $d \geq 1$

$$A_d\begin{pmatrix}X_1,\ldots,X_d\\Y_1,\ldots,Y_d\end{pmatrix} = \sum_{\substack{k_1,\ldots,k_d\geq 1\\m_1,\ldots,m_d\geq 0}} \varphi_*(y_{k_1,m_1}\ldots y_{k_d,m_d})X_1^{k_1-1}\frac{Y_1^{m_1}}{m_1!}\ldots X_d^{k_d-1}\frac{Y_d^{m_d}}{m_d!}.$$

As before, we will call φ_* the coefficient map of A.

Denote by $\mathrm{BARI}_{\mathrm{il}}^{\mathrm{pow},R}$ (resp. $\mathrm{ARI}_{\mathrm{il}}^{\mathrm{pow},R}$) the subspace of all alternil bimoulds (resp. moulds).

So a bimould $A \in \mathrm{BARI}^{\mathrm{pow},R}$ is alternil with coefficient map φ_* if and only if for all $0 < n < d$

$$\varphi_*\left(\rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_1,\ldots,X_n\\Y_1,\ldots,Y_n\end{pmatrix} * \rho_{\mathcal{Y}^{\mathrm{bi}}}(\mathcal{W})\begin{pmatrix}X_{n+1},\ldots,X_d\\Y_{n+1},\ldots,Y_d\end{pmatrix}\right) = 0. \tag{C.17.1}$$

Remark C.18. Similar to the case of symmetrality and symmetrility, one could define alternality and alternility for (bi-)moulds by the explicit formulas obtained from (C.16.1) and (C.17.1). This allows to extend these symmetries to wider classes of (bi-)moulds like $\mathrm{BARI}^{\mathrm{fL},R}$.

Alternality can be seen as the associated depth-graded property to alternility.

Proposition C.19. *Let $r \geq 1$ and $A = (0,0,\ldots,0,A_r,A_{r+1},\ldots)$ be an alternil bimould. Then $\mathrm{gr}_D\, A = (0,0,\ldots,0,A_r,0,0,\ldots)$ is an alternal bimould.*

Proof. From Corollary A.76 and A.77, we deduce that the explicit formulas for alternality (C.16.1) and alternility (C.17.1) in some depth d differ only by terms of depth $< d$. In particular, the bimould $\mathrm{gr}_D\, A$ is simultaneously alternil and alternal. □

C.2 (Bi-)Moulds and Lie algebras

This subsection is devoted to present the basic Lie algebra structure on the subspaces $\mathrm{ARI}_{\mathrm{al}}$ and $\mathrm{BARI}_{\mathrm{al}}$. In the following, we work over some fixed commutative $\mathbb{Q}$-algebra R with unit.

Decompose $\mathbf{w} = \binom{X_1,\dots,X_d}{Y_1,\dots,Y_d}$ into $\mathbf{w} = \mathbf{abc}$, where

$$\mathbf{a} = \begin{pmatrix} X_1,\dots,X_k \\ Y_1,\dots,Y_k \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} X_{k+1},\dots,X_{k+l} \\ Y_{k+1},\dots,Y_{k+l} \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} X_{k+l+1},\dots,X_d \\ Y_{k+l+1},\dots,Y_d \end{pmatrix}.$$

The flexions are defined by $\mathbf{a}\rfloor = \mathbf{a}$ if $\mathbf{b} = \emptyset$, $\lceil\mathbf{b} = \mathbf{b}$ if $\mathbf{a} = \emptyset$, $\mathbf{b}\rceil = \mathbf{b}$ if $\mathbf{c} = \emptyset$, $\lfloor\mathbf{c} = \mathbf{c}$ if $\mathbf{b} = \emptyset$, and

$$\mathbf{a}\rfloor = \begin{pmatrix} X_1,\dots,X_k \\ Y_1,\dots,Y_{k-1},Y_k+\dots+Y_{k+l} \end{pmatrix}, \qquad \lceil\mathbf{b} = \begin{pmatrix} X_{k+1}-X_k,\dots,X_{k+l}-X_k \\ Y_{k+1},\dots,Y_{k+l} \end{pmatrix},$$

$$\mathbf{b}\rceil = \begin{pmatrix} X_{k+1}-X_{k+l+1},\dots,X_{k+l}-X_{k+l+1} \\ Y_{k+1},\dots,Y_{k+l} \end{pmatrix}, \qquad \lfloor\mathbf{c} = \begin{pmatrix} X_{k+l+1},\dots,X_d \\ Y_{k+1}+\dots+Y_{k+l+1},Y_{k+l+2},\dots,Y_d \end{pmatrix}.$$

Definition C.20. For $A, B \in \mathrm{BARI}$, define the derivation (with respect to mu) arit_B by

$$\mathrm{arit}_B(A)(\mathbf{w}) = \sum_{\substack{\mathbf{w}=\mathbf{abc} \\ \mathbf{b},\mathbf{c}\neq\emptyset}} A(\mathbf{a}\lfloor\mathbf{c})B(\mathbf{b}\rceil) - \sum_{\substack{\mathbf{w}=\mathbf{abc} \\ \mathbf{a},\mathbf{b}\neq\emptyset}} A(\mathbf{a}\rfloor\mathbf{c})B(\lceil\mathbf{b}).$$

Example C.21. For bimoulds $A, B \in \mathrm{BARI}$, one computes

$$\mathrm{arit}_B(A)\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2 \end{pmatrix} = A\begin{pmatrix} X_2 \\ Y_1+Y_2 \end{pmatrix} B\begin{pmatrix} X_1-X_2 \\ Y_1 \end{pmatrix} - A\begin{pmatrix} X_1 \\ Y_1+Y_2 \end{pmatrix} B\begin{pmatrix} X_2-X_1 \\ Y_2 \end{pmatrix},$$

$$\begin{aligned}
\mathrm{arit}_B(A)\begin{pmatrix} X_1,X_2,X_3 \\ Y_1,Y_2,Y_3 \end{pmatrix} &= A\begin{pmatrix} X_1,X_3 \\ Y_1,Y_2+Y_3 \end{pmatrix} B\begin{pmatrix} X_2-X_3 \\ Y_2 \end{pmatrix} \\
&+ A\begin{pmatrix} X_3 \\ Y_1+Y_2+Y_3 \end{pmatrix} B\begin{pmatrix} X_1-X_3,X_2-X_3 \\ Y_1,Y_2 \end{pmatrix} + A\begin{pmatrix} X_2,X_3 \\ Y_1+Y_2,Y_3 \end{pmatrix} B\begin{pmatrix} X_1-X_2 \\ Y_1 \end{pmatrix} \\
&- A\begin{pmatrix} X_1,X_3 \\ Y_1+Y_2,Y_3 \end{pmatrix} B\begin{pmatrix} X_2-X_1 \\ Y_2 \end{pmatrix} - A\begin{pmatrix} X_1,X_2 \\ Y_1,Y_2+Y_3 \end{pmatrix} B\begin{pmatrix} X_3-X_2 \\ Y_3 \end{pmatrix} \\
&- A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3 \end{pmatrix} B\begin{pmatrix} X_2-X_1,X_3-X_1 \\ Y_2,Y_3 \end{pmatrix},
\end{aligned}$$

$$\begin{aligned}
\mathrm{arit}_B(A)\begin{pmatrix} X_1,X_2,X_3,X_4 \\ Y_1,Y_2,Y_3,Y_4 \end{pmatrix} &= A\begin{pmatrix} X_4 \\ Y_1+Y_2+Y_3+Y_4 \end{pmatrix} B\begin{pmatrix} X_1-X_4,X_2-X_4,X_3-X_4 \\ Y_1,Y_2,Y_3 \end{pmatrix} \\
&+ A\begin{pmatrix} X_3,X_4 \\ Y_1+Y_2+Y_3,Y_4 \end{pmatrix} B\begin{pmatrix} X_1-X_3,X_2-X_3 \\ Y_1,Y_2 \end{pmatrix} + A\begin{pmatrix} X_2,X_3,X_4 \\ Y_1+Y_2,Y_3,Y_4 \end{pmatrix} B\begin{pmatrix} X_1-X_2 \\ Y_1 \end{pmatrix} \\
&+ A\begin{pmatrix} X_1,X_2,X_4 \\ Y_1,Y_2,Y_3+Y_4 \end{pmatrix} B\begin{pmatrix} X_3-X_4 \\ Y_3 \end{pmatrix} + A\begin{pmatrix} X_1,X_4 \\ Y_1,Y_2+Y_3+Y_4 \end{pmatrix} B\begin{pmatrix} X_2-X_4,X_3-X_4 \\ Y_2,Y_3 \end{pmatrix} \\
&+ A\begin{pmatrix} X_1,X_3,X_4 \\ Y_1,Y_2+Y_3,Y_4 \end{pmatrix} B\begin{pmatrix} X_2-X_3 \\ Y_2 \end{pmatrix} - A\begin{pmatrix} X_1,X_2,X_4 \\ Y_1,Y_2,Y_3+Y_4 \end{pmatrix} B\begin{pmatrix} X_4-X_3 \\ Y_4 \end{pmatrix}
\end{aligned}$$

$$
\begin{aligned}
&- A\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2+Y_3+Y_4 \end{pmatrix} B\begin{pmatrix} X_3-X_2, X_4-X_2 \\ Y_3, Y_4 \end{pmatrix} \\
&- A\begin{pmatrix} X_1 \\ Y_1+Y_2+Y_3+Y_4 \end{pmatrix} B\begin{pmatrix} X_2-X_1, X_3-X_1, X_4-X_1 \\ Y_2, Y_3, Y_4 \end{pmatrix} \\
&- A\begin{pmatrix} X_1, X_2, X_4 \\ Y_1, Y_2+Y_3, Y_4 \end{pmatrix} B\begin{pmatrix} X_3-X_2 \\ Y_3 \end{pmatrix} - A\begin{pmatrix} X_1, X_4 \\ Y_1+Y_2+Y_3, Y_4 \end{pmatrix} B\begin{pmatrix} X_2-X_1, X_3-X_1 \\ Y_2, Y_3 \end{pmatrix} \\
&- A\begin{pmatrix} X_1, X_3, X_4 \\ Y_1+Y_2, Y_3, Y_4 \end{pmatrix} B\begin{pmatrix} X_2-X_1 \\ Y_2 \end{pmatrix}.
\end{aligned}
$$

Definition C.22. For two bimoulds $A, B \in \mathrm{BARI}$, set

$$\mathrm{preari}(A,B) = \mathrm{arit}_A(B) + \mathrm{mu}(B,A).$$

Then, the ari bracket is defined as

$$\mathrm{ari}(A,B) = \mathrm{preari}(A,B) - \mathrm{preari}(B,A).$$

Example C.23. For two bimoulds $A, B \in \mathrm{BARI}$, one obtains

$$
\begin{aligned}
\mathrm{ari}(A,B)\begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} &= B\begin{pmatrix} X_2 \\ Y_1+Y_2 \end{pmatrix} A\begin{pmatrix} X_1-X_2 \\ Y_1 \end{pmatrix} - B\begin{pmatrix} X_1 \\ Y_1+Y_2 \end{pmatrix} A\begin{pmatrix} X_2-X_1 \\ Y_2 \end{pmatrix} \\
&- A\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} B\begin{pmatrix} X_2 \\ Y_2 \end{pmatrix} - A\begin{pmatrix} X_2 \\ Y_1+Y_2 \end{pmatrix} B\begin{pmatrix} X_1-X_2 \\ Y_1 \end{pmatrix} \\
&+ A\begin{pmatrix} X_1 \\ Y_1+Y_2 \end{pmatrix} B\begin{pmatrix} X_2-X_1 \\ Y_2 \end{pmatrix} + B\begin{pmatrix} X_1 \\ Y_1 \end{pmatrix} A\begin{pmatrix} X_2 \\ Y_2 \end{pmatrix},
\end{aligned}
$$

In difference to the previous cases, one obtains the definition of the ari bracket on the space ARI of moulds by considering just the variables Y_i. For example, one has for $A, B \in \mathrm{ARI}$

$$
\begin{aligned}
\mathrm{ari}(A,B)(X_1,X_2) = B(X_1+X_2)A(X_1) &- B(X_1+X_2)A(X_2) - A(X_1)B(X_2) \\
&- A(X_1+X_2)B(X_1) + A(X_1+X_2)B(X_2) + B(X_1)A(X_2).
\end{aligned}
$$

Combining both statements in [SS20, Theorem 3.1.], one obtains the following.

Theorem C.24. *The spaces* $\mathrm{BARI}_{\mathrm{al}}$ *and* $\mathrm{ARI}_{\mathrm{al}}$ *equipped with the ari bracket are Lie algebras.* □

Define

$$
\begin{aligned}
\mathrm{ARI}^{\mathrm{pol},R} &= \left\{ A \in \mathrm{ARI} \;\middle|\; \begin{array}{l} \cdot\ A_d(X_1,\dots,X_d) \in R[X_1,\dots,X_d] \text{ for all } d \geq 1, \\ \cdot\ A_d(X_1,\dots,X_d) \neq 0 \text{ only for finitely many } d \geq 1 \end{array} \right\}, \\
\mathrm{BARI}^{\mathrm{pol},R} &= \left\{ A \in \mathrm{BARI} \;\middle|\; \begin{array}{l} \cdot\ A_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} \in R[X_1,Y_1,\dots,X_d,Y_d] \text{ for all } d \geq 1, \\ \cdot\ A_d\begin{pmatrix} X_1,\dots,X_d \\ Y_1,\dots,Y_d \end{pmatrix} \neq 0 \text{ only for finitely many } d \geq 1 \end{array} \right\},
\end{aligned}
$$

and similarly for all subspaces of ARI^R and BARI^R. The two spaces $\mathrm{ARI}^{\mathrm{pol},R}$ and $\mathrm{BARI}^{\mathrm{pol},R}$ are bi-graded by weight and depth, the homogeneous component of weight w is given by

$$\left(\mathrm{(B)ARI}^{\mathrm{pol},R}\right)^{(w)} = \left\{ A \in \mathrm{(B)ARI}^{\mathrm{pol},R} \;\middle|\; \begin{array}{l} A_d \text{ homogeneous of degree } w-d \\ \text{for all } d \geq 1 \end{array} \right\} \qquad \text{(C.24.1)}$$

and the homogeneous component of weight w and depth d is given by

$$\Big((\mathrm{B})\mathrm{ARI}^{\mathrm{pol},R}\Big)^{(w,d)} = \left\{ A \in (\mathrm{B})\mathrm{ARI}^{\mathrm{pol},R} \;\middle|\; \begin{array}{l} \cdot\ A = (\overbrace{0,\ldots,0}^{d-1}, A_d, 0, \ldots), \\ \cdot\ A_d \text{ homogeneous of degree } w-d. \end{array} \right\}. \tag{C.24.2}$$

Since the ari bracket is defined by a finite number of terms homogeneous in weight and depth, Theorem C.24 implies the following.

Corollary C.25. *Both* $\mathrm{ARI}_{\mathrm{al}}^{\mathrm{pol}}$ *and* $\mathrm{BARI}_{\mathrm{al}}^{\mathrm{pol}}$ *are bi-graded Lie algebras with the ari bracket.*

Remark C.26. The set of all symmetral (bi-)moulds is the corresponding Lie group to the alternal (bi-)moulds. Define for any bimould $A \in \mathrm{BARI}$,

$$\begin{aligned} \mathrm{expari}(A) &= \sum_{n\geq 0} \frac{1}{n!} \underbrace{\mathrm{preari}(\ldots\mathrm{preari}(\mathrm{preari}(A,A),A),\ldots,A)}_{n-1 \text{ times}} \\ &= 1 + A + \frac{1}{2}\,\mathrm{preari}(A,A) + \frac{1}{6}\,\mathrm{preari}(\mathrm{preari}(A,A),A) + \ldots\ . \end{aligned} \tag{C.26.1}$$

By [Sc15, Proposition 2.6.1.] the operator expari restricts to bijections

$$\mathrm{expari} : \mathrm{BARI}_{\mathrm{al}} \to \mathrm{GBARI}_{\mathrm{as}}, \qquad \mathrm{expari} : \mathrm{ARI}_{\mathrm{al}} \to \mathrm{GARI}_{\mathrm{as}}\,.$$

In particular, both sets $\mathrm{GBARI}_{\mathrm{as}}$ and $\mathrm{GARI}_{\mathrm{as}}$ are groups, the explicit group law gari is given in [Sc15, (2.7.3.)].

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Abstract

We study the algebraic structure of multiple q-zeta values, being inspired by the theory of multiple zeta values.

Multiple zeta values are real numbers, which occur and have been studied in various areas of mathematics and high energy physics. They satisfy a lot of algebraic relations and conjecturally all of those arise from the so-called extended double shuffle relations. This leads to the definition of the algebra $\mathcal{Z}^f$ of formal multiple zeta values, which was for example studied by Ihara-Kaneko-Zagier or Gangl-Kaneko-Zagier. In his thesis, Racinet gave an algebraic approach to the formal multiple zeta values in terms of non-commutative power series. More precisely, he showed that the algebra $\mathcal{Z}^f$ modulo $\zeta^f(2)$ represents a pro-unipotent affine group scheme DM_0. Using the corresponding Lie algebra $\mathfrak{dm}_0$ allowed him to prove that $\mathcal{Z}^f$ is a free polynomial algebra. Moreover, one obtains that $\mathcal{Z}^f$ equipped with Goncharov's coproduct is a Hopf algebra. The appendix provides a detailed exposition of this approach.

A multiple q-zeta value is a particular kind of q-series, which yields a multiple zeta value for the limit $q \to 1$ (whenever the corresponding multiple zeta value exists). We introduce the balanced multiple q-zeta values, which span the algebra $\mathcal{Z}_q$ of all multiple q-zeta values and satisfy very explicit and simple relations. In particular, their product formula is a balanced combination of the two product formulas for multiple zeta values. Another advantage of the balanced multiple q-zeta values is that they give a simple description of a conjectural weight-grading on $\mathcal{Z}_q$, which extends the weight-grading of the quasi-modular forms. Moreover, the balanced multiple q-zeta values are closely related to the combinatorial multiple Eisenstein series, which were obtained in a joint work with Bachmann.

With similar techniques as for multiple zeta values, we extend the balanced multiple q-zeta values to a wider set of indices, such that they lie in the image of some morphism from a quasi-shuffle algebra. The expected relations for these regularized multiple q-zeta values lead to the definition of the algebra $\mathcal{Z}_q^f$ of formal multiple q-zeta values. This thesis provides an algebraic approach to the algebra $\mathcal{Z}_q^f$, which should be seen as a q-analog of Racinet's approach to formal multiple zeta values.

It turns out that the algebra $\mathcal{Z}_q^f$ modulo the formal quasi-modular forms $\zeta_q^f(2)$, $\zeta_q^f(4), \zeta_q^f(6)$ represents an affine scheme BM_0, which has values in a completed Hopf algebra of non-commutative power series. Moreover, the affine group scheme DM_0 introduced by Racinet for the formal multiple zeta values embeds into BM_0. This implies a projection from the algebra $\mathcal{Z}_q^f$ of formal multiple q-zeta values onto the algebra $\mathcal{Z}^f$ of formal multiple zeta values, which should be seen as a formal version of the limit $q \to 1$.

Linearizing the defining equations of the affine scheme BM_0 leads to a space $\mathfrak{bm}_0$ consisting of non-commutative polynomials. In analogy to the case of multiple zeta values, we expect that BM_0 is a pro-unipotent affine group scheme and $\mathfrak{bm}_0$ is its Lie algebra. The space $\mathfrak{bm}_0$ is very explicit and its generators can be computed up to weight 13, this allows testing potential Lie brackets on $\mathfrak{bm}_0$.

In this thesis, we obtained a Lie algebra $\mathfrak{mq}$ equipped with the so-called q-Ihara bracket $\{-,-\}_q$, which is a generalization of the twisted Magnus Lie algebra $(\mathfrak{mt}, \{-,-\})$. Just as $\mathfrak{dm}_0$ is a Lie subalgebra of the twisted Magnus Lie algebra, we expect that $\mathfrak{bm}_0$ is a Lie subalgebra of $(\mathfrak{mq}, \{-,-\}_q)$. The elements in $\mathfrak{bm}_0$ as well as the q-Ihara bracket $\{-,-\}_q$

are quite complicated. By computer experiments, we verified that the q-Ihara bracket preserves $\mathfrak{bm}_0$ up to weight 9, and with some more effort one could probably extend this to weight 13.

On the other hand, Kühn proposed an approach to Lie algebras related to multiple q-zeta values by using Ecalle's theory of (bi-)moulds. We show that the (conjectural) Lie algebra of alternil and swap invariant bimoulds is isomorphic to $\mathfrak{bm}_0$. Although the alternil and swap invariant bimoulds can only be calculated in very small weights and depths, since the occurring bimoulds become very large, its depth-graded version is much more accessible for explicit calculations. Therefore, the bimould approach as well as the non-commutative approach to Lie algebras related to multiple q-zeta values are both of interest.

Independent of the general algebraic approach to multiple q-zeta values explained before, explicit calculations give a partial result towards Bachmann's conjecture that the brackets and the bi-brackets span the same space. This result is a side product of this thesis.

In summary, this thesis opens up a lot of new questions and possible ways to continue, some of which are described at the end of the introduction.

Zusammenfassung

Wir untersuchen die algebraische Struktur der multiplen q-Zetawerte inspiriert durch die Theorie der multiplen Zetawerte.

Multiple Zetawerte sind reelle Zahlen, welche in diversen Feldern der Mathematik und der Hochenergiephysik auftreten und studiert werden. Sie erfüllen eine Vielzahl von algebraischen Relationen und vermutungsweise entstehen alle durch die sogenannten erweiterten Doppelshuffle-Relationen. Dies führt zu der Definition der Algebra $\mathcal{Z}^f$ der formalen multiplen Zetawerte, welche zum Beispiel von Ihara-Kaneko-Zagier oder Gangl-Kaneko-Zagier studiert wurde. Racinet erklärt in seiner Doktorarbeit einen algebraischen Zugang zu den formalen multiplen Zetawerten, der nicht-kommutative Potenzreihen nutzt. Genauer zeigt er, dass die Algebra $\mathcal{Z}^f$ modulo $\zeta^f(2)$ ein pro-unipotentes affines Gruppenschema DM_0 repräsentiert. Dann nutzt er die zugehörige Lie-Algebra $\mathfrak{dm}_0$ um zu zeigen, dass $\mathcal{Z}^f$ eine freie Polynomalgebra ist. Außerdem folgt, dass $\mathcal{Z}^f$ ausgestattet mit Goncharovs Koprodukt eine Hopf-Algebra ist. Der Appendix enthält eine detaillierte Darstellung dieses Zugangs.

Ein multipler q-Zetawert ist eine spezielle Art einer q-Reihe, welche unter dem Grenzwert $q \to 1$ einen multiplen Zetawert liefert (wenn der zugehörige multiple Zetawert existiert). Wir führen die balancierten multiplen q-Zetawerte ein, welche die Algebra $\mathcal{Z}_q$ aufspannen und sehr explizite und einfache Relationen erfüllen. Insbesondere ist ihre Produktformel eine ausbalancierte Kombination der beiden Produktformeln für multiple Zetawerte. Ein weiterer Vorteil der balancierten multiplen q-Zetawerte ist, dass sie eine einfache Beschreibung einer vermuteten Gewichtsgraduierung auf $\mathcal{Z}_q$ liefern, welche die Gewichtsgraduierung der Quasi-Modulformen erweitert. Die balancierten multiplen q-Zetawerte stehen in engem Zusammenhang zu den kombinatorischem multiplen Eisensteinreihen, welche in einer gemeinsamen Arbeit mit Bachmann entdeckt wurden.

Mit ähnlichen Methoden wie bei den multiplen Zetawerten, erweitern wir die balancierten multiplen q-Zetawerte auf eine größere Menge von Indices, sodass diese im Bild eines Morphismus von einer Quasishuffle-Algebra liegen. Die erwarteten Relationen von diesen regularisierten multiplen q-Zetawerten liefern die Definition der Algebra $\mathcal{Z}_q^f$ der formalen multiplen q-Zetawerte. Diese Arbeit präsentiert einen algebraischen Zugang zu der Algebra $\mathcal{Z}_q^f$, welcher als q-Analog von Racinet's Zugang zu den formalen multiplen Zetawerten gesehen werden sollte.

Es stellt sich heraus, dass die Algebra $\mathcal{Z}_q^f$ modulo den formalen Quasi-Modulformen $\zeta_q^f(2)$, $\zeta_q^f(4)$, $\zeta_q^f(6)$ ein affines Schema BM_0 darstellt, welches Werte in einer komplettierten Hopf-Algebra von nicht-kommutativen Potenzreihen hat. Darüber hinaus gibt es eine Einbettung des affinen Gruppenschemas DM_0, welches von Racinet für die formalen multiplen Zetawerte eingeführt wurde, in das affine Schema BM_0. Dies impliziert eine Projektion von der Algebra $\mathcal{Z}_q^f$ der formalen multiplen q-Zetawerte auf die Algebra $\mathcal{Z}^f$ der formalen multiplen Zetawerte, welche als formale Version der Grenzwertabbildung $q \to 1$ gesehen werden sollte.

Linearisieren der definierenden Gleichungen des affinen Schemas BM_0 führt zu dem Vektorraum $\mathfrak{bm}_0$, der aus nicht-kommutativen Polynomen besteht. In Analogie zu den multiplen Zetawerten erwarten wir, dass BM_0 ein pro-unipotentes affines Gruppenschema ist und $\mathfrak{bm}_0$ die zugehörige Lie-Algebra. Der Vektorraum $\mathfrak{bm}_0$ ist sehr explizit und die Erzeuger können bis zum Gewicht 13 berechnet werden, dies erlaubt potentielle Lie-Klammern auf

$\mathfrak{bm}_0$ zu testen.

In dieser Arbeit präsentieren wir eine Lie-Algebra $\mathfrak{mq}$ ausgestattet mit der sogenannten q-Ihara-Klammer $\{-,-\}_q$, welche eine Verallgemeinerung der getwisteten Magnus Lie-Algebra $(\mathfrak{mt}, \{-,-\})$ ist. Genauso wie $\mathfrak{dm}_0$ eine Lie-Unteralgebra der getwisteten Magnus Lie-Algebra ist, erwarten wir, dass $\mathfrak{bm}_0$ eine Lie-Unteralgebra von $(\mathfrak{mq}, \{-,-\}_q)$ ist. Die Elemente in $\mathfrak{bm}_0$ und die q-Ihara-Klammer $\{-,-\}_q$ sind recht kompliziert. Mit Computer-Experimenten konnten wir verifizieren, dass $\mathfrak{bm}_0$ abgeschlossen unter der q-Ihara-Klammer ist bis zum Gewicht 9, mit etwas mehr Aufwand kann dies vermutlich bis Gewicht 13 fortgeführt werden.

Auf der anderen Seite hat Kühn einen Zugang zu Lie-Algebren von multiplen q-Zetawerten vorgeschlagen, welcher Ecalles Theorie der (Bi-)Moulds nutzt. Wir zeigen, dass die (vermutete) Lie-Algebra der alternil und swap-invarianten Bimoulds isomorph ist zu $\mathfrak{bm}_0$. Obwohl alternil und swap-invariant Bimoulds nur in sehr kleinen Gewichten und Tiefen berechnet werden können, da die auftretenden Bimoulds sehr groß sind, ist die tiefengraduierte Version wesentlich zugänglicher für explizite Berechnungen. Daher ist sowohl der Zugang via Bimoulds als auch der nicht-kommutative Zugang zu Lie-Algebren von multiplen q-Zetawerten sehr interessant.

Unabhängig von dem oben erklärten algebraischen Zugang zu multiplen q-Zetawerten liefern explizite Berechnungen Teilresultate in Richtung Bachmanns Vermutung, dass die Klammern und die Bi-Klammern denselben Vektorraum aufspannen. Dieses Resultat ist einer Nebenprodukt dieser Doktorarbeit.

Zusammenfassend wirft diese Arbeit viele neue Fragen auf und liefert viele mögliche Wege zur Fortsetzung, ein paar von diesen werden am Ende der Einleitung beschrieben.

Publications related to this dissertation

Subsection 2.5 is based on

[BB22] H. Bachmann, A. Burmester. ”Combinatorial multiple Eisenstein series”. Preprint, *ArXiv: 2203.17074v2 [math.NT], 2022.*

The paper provides the construction of the combinatorial (bi-)multiple Eisenstein series and presents their properties. H. Bachmann and I independently obtained a construction for the combinatorial bi-multiple Eisenstein series in depth 3, therefore we decided to study the general depth case together. The main idea for the general construction is due to H. Bachmann and together we figured out the details. Then my main task was to find a proof that this construction has indeed the desired properties. H. Bachmann came up with a first draft of the paper, which we then filled in together with details.

Eidesstattliche Versicherung

Hiermit erkläre ich an Eides statt, dass ich die vorliegende Dissertationsschrift selbst verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe.

Hamburg, den 01.12.2022