Master's Thesis

Computing the single-valued Knizhnik-Zamolodchikov associator

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1 Introduction

In the 1980s V. Drinfel'd developed the theory of Drinfel'd associators; algebraic objects that provide a natural generalization of the classical concept of exponential functions, which have long played a fundamental role in many areas of mathematics. Drinfel'd associators have applications in a wide range of fields, including algebraic geometry, topology, deformation quantization and are closely related to the theory of quantum groups, which are a class of non-commutative algebraic structures that arose in the context of mathematical physics and have since found applications in many areas of mathematics. They also have deep connections to the theory of operads, which provide a powerful language for studying algebraic structures with composition.

Drinfel'd himself introduced two associators in [11] the Knizhnik-Zamolodchikov (KZ) associator Φ_{KZ} and the anti-KZ associator $\Phi_{\overline{KZ}}$ (see Section 2.5). In [1] Alekseev and Torossian introduced another associator the eponymous Alekseev-Torossian (AT) associator Φ_{AT} which was later shown by Ševera and Willwacher to be a Drinfel'd associator. In [18] Rossi and Willwacher constructed a family of Drinfel'd associators interpolating between the KZ-associator, the AT-associator and the anti-KZ-associator that is they proved the following:

Theorem 1.1. *There is a family of Drinfel'd associators Φ^t over $\mathbb{C}$ and odd degree elements $\{\tau_3, \tau_5, \ldots\}$ of $\mathfrak{grt}_1$, such that*

$$\Phi^0 = \Phi_{KZ} \qquad \Phi^{\frac{1}{2}} = \Phi_{AT} \qquad \Phi^1 = \Phi_{\overline{KZ}}$$

and

$$\partial_t \Phi^t = \tau^t \cdot \Phi^t$$

where

$$\tau^t := \sum_{j=1}^{\infty} (t(1-t))^{2j} \tau_{2j+1} \in \mathfrak{grt}_1.$$

Here $\mathfrak{grt}_1$ denotes the Grothendieck-Teichmüller Lie algebra (see Section 2.5). The associators Φ^t can then explicitly be given by

$$\Phi^t = \mathcal{P}\exp\left(\int_0^t \tau^s \,\mathrm{d}s\right) \cdot \Phi_{KZ}$$

where $\mathcal{P}\exp$ is the path ordered exponential, which is defined as a sum of iterated integrals:

$$\mathcal{P}\exp\left(\int_0^t \tau^s \,\mathrm{d}s\right) := 1 + \int_0^t \tau^s \,\mathrm{d}s + \int_0^t \tau^{s_1}\left(\int_0^{s_1} \tau^{s_2}\,\mathrm{d}s_2\right)\mathrm{d}s_1 + \int_0^t \tau^{s_1}\left(\int_0^{s_1} \tau^{s_2}\left(\int_0^{s_2} \tau^{s_3}\,\mathrm{d}s_3\right)\mathrm{d}s_2\right)\mathrm{d}s_1 + \ldots$$

Further, they give an explicit formula to calculate τ^t via the Kontsevich graph complex GC (see Section 4.1). That is,

$$\tau_{2j+1} = \sum_{\Gamma} \frac{c_\Gamma}{|\mathrm{Aut}(\Gamma)|}\phi(\Gamma)$$

where the sum is over all isomorphism classes of graphs in GC with $2j+2$ vertices. Here, ϕ is a map from $\phi : \mathsf{GC} \to \mathfrak{sder}_2$ (see Section 4.5) with $\mathfrak{sder}_k$ being the space of special derivations (see Section 4.3) and c_Γ is given by

$$c_\Gamma := \int_{\mathbb{C}^{2j}} \sum_{\substack{e,e' \in E(\Gamma) \\ e \neq e'}} (-1)^{o(e,e')} \frac{1}{\pi i} \log\left|z_{s(e')} - z_{t(e')}\right| \bigwedge_{e'' \in E(\Gamma)\setminus\{e,e'\}} \frac{1}{\pi i} d\log\left|z_{s(e'')} - z_{t(e'')}\right|. \tag{1}$$

Here the product over the edges shall be taken in their order and $o(e', e)$ is $e' + e - 1$ for $e' < e$ and $e' + e$ else. Let us further denote by ψ the following element of the Grothendieck-Teichmüller group GRT_1 (see Section 2.5):

$$\psi := \mathcal{P}\exp\left(\int_0^1 \tau^s \,\mathrm{d}s\right).$$

In [7] Brown showed the following result, whose implications for the above construction have not been studied until now:

Theorem 2.13.

$$\Phi_{KZ}^{\mathrm{sv}} = \mathcal{L}(1) = \psi$$

Here $\mathcal{L}(1)$ denotes the generating series of the single-valued polylogarithms evaluated at 1 and Φ_{KZ}^{sv} denotes the single-valued KZ-associator (see Section 2.3). From this it follows that all coefficients in the series expansion of ψ are single-valued multiple zeta values (MZVs). This, for example, instantly answers the question of the irrationality of the AT-associator as shown in a lengthy computation by M. Felder in [12]. The argument using single-valuedness goes as follows: As all coefficients of ψ are single-valued MZVs we know that all non-single-valued MZVs, for example $\zeta(5,3)$, do not appear in any of those coefficients. However, as $\zeta(5,3)$ appears in Φ_{KZ} it follows that $\zeta(5,3)$ also appears in Φ_{AT} as

$$\Phi_{AT} = \mathcal{P}\exp\left(\int_0^{\frac{1}{2}} \tau^s \mathrm{d}s\right) \cdot \Phi_{KZ}.$$

From this the irrationality follows as $\frac{\zeta(5,3)}{\pi^8}$ is, conjecturally, irrational. On a side note, from either [2] by Banks, Panzer and Pym, [8] by Brown and Dupont or [21] by Vanhove and Zerbini it also follows that the c_Γ have single-valued MZV coefficients and thus that the coefficients of ψ are single-valued MZVs. Using the single-valued integration as described in [2] we calculate the coefficients c_Γ for the wheel graphs in Section 2.4 and find:

Theorem 2.16. *Let $V \in \mathbb{N}$ and denote by Γ the wheel graph on $V+1$ vertices as described in Figure 2. Then for even V, $c_\Gamma = 0$ and for $V = 2k+1$ odd it holds that*

$$c_\Gamma = 2(4k+1)\binom{4k}{2k}\frac{\zeta(2k+1)}{(2\pi i)^{2k+1}}.$$

In principle, this result was already known by M. Felder's calculations of c_{2n} in [12] or Merkulov's calculations in [17, Appendix 1] and using the various connections between deformation quantization, Drinfel'd associators and GC. However, the specific calculation of the c_Γ via its integral definition has, to the best of our knowledge, not been done before.

Afterward we turn to the calculation of the τ_{2j+1}. Using the Lyndon basis expansion we find for the τ_{2j+1} up to depth 3:

$$\tau_{2j+1} = c_{2j}\,\mathrm{ad}_x^{2j}(y) + \sum_{\substack{0\le\alpha<\beta\\ \alpha+\beta=2j-1}} c_{\alpha,\beta}\left[\mathrm{ad}_x^{\alpha}(y), \mathrm{ad}_x^{\beta}(y)\right] + \sum_{\substack{\beta<\gamma,\alpha\le\gamma\\ \alpha+\beta+\gamma=2j-2}} c_{\alpha,\beta,\gamma}\left[\mathrm{ad}_x^{\alpha}(y), \left[\mathrm{ad}_x^{\beta}(y), \mathrm{ad}_x^{\gamma}(y)\right]\right]$$

Picking up on the idea by M. Felder in [12] to consider the equation $\psi \cdot \Phi_{KZ} = \Phi_{\overline{KZ}}$ we recover the coefficients $c_{2n}, c_{\alpha,\beta}$ and $c_{\alpha,\beta,\gamma}$. For the first two explicit formulas can be given

$$c_{2n} = 2(4n+1)\binom{4n}{2n}\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}$$

as shown by M. Felder in [12] and for depth 2 we find

Theorem 3.5. *Let $n \in \mathbb{N}$ and let $\alpha \in \{0, \dots, n-1\}$ and $\beta = 2n-1-\alpha$. Then the following holds:*

$$c_{\alpha,\beta} = \frac{-(4n+1)!}{((2n)!)^2}\left(\binom{2n}{\alpha} - \binom{2n}{\alpha+1} + (-1)^{\alpha+1}\right)\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}.$$

For depth 3 we found an implicit formula as described in Theorem 3.14 and implemented it in Python as described in Appendix C. For small weights, tables of the coefficients $c_{\alpha,\beta,\gamma}$ can be found at the end of the work in Appendix D. Using the above formulas, we implemented the calculation of Φ_{AT} as well as all other associators Φ^t from Theorem 1.1 up to depth 3 and give the coefficients of Φ_{AT} for depth 3 for the smallest weights at the end of Section 3.3. Formulas for the coefficients of Φ_{AT} for depth 1 and 2 can be found in [12]. Moreover, we show the following for Φ_{AT} :

Theorem 3.15. *Let $w = x^{k_1}y \dots yx^{k_n}$. Then if $|w|$ is odd $\Phi_{AT}(w) = 0$, that is Φ_{AT} vanishes on odd words.*

Using Theorem 2.13 and Theorem 3.5 we find the following explicit formulas for the single-valued MZVs in depth 2:

Theorem 2.14. *Let $w = x^a yx^b yx^c$ be a word of depth 2 of odd length $|w| = 2n+1$. Then we have that*

$$\frac{\zeta_{\text{sv}}(w)}{(2\pi i)^{|w|}} = \left((-1)^{a+1}\binom{2n}{a} + (-1)^b\binom{2n}{b} + (-1)^{c+1}\binom{2n}{c}\right)\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}.$$

as well as

Theorem 2.15. *Let $w = x^a yx^b yx^c$ be a word of depth 2 of even length $|w| = 2n$. Then we have*

$$\frac{\zeta_{\text{sv}}(w)}{(2\pi i)^{|w|}} = 4\sum_{l+m=n-1}\left((-1)^{a+c}\binom{2l}{a}\binom{2m}{c} + (-1)^{a+b}\binom{2l}{b}\binom{2m}{a}\right.$$
$$\left. -(-1)^{b+c}\binom{2l}{b}\binom{2m}{c}\right)\frac{\zeta(2l+1)\zeta(2m+1)}{(2\pi i)^{2n}}.$$

Taking a detour, we turn to the map $\phi : \mathsf{GC} \to \mathfrak{sder}_2$ which descends to an isomorphism from $H^0(\mathsf{GC})$ to $\mathfrak{grt}_1$ as introduced by Willwacher in [22] and improved upon by Rossi and Willwacher in [18]. In Section 4 we introduce the necessary theory behind the map and give a detailed explanation of its working. We also implemented this map in Python and could thus calculate the $\mathfrak{grt}_1$ elements corresponding to the cocycles in degree 3, 5 and 7. For degree 3 the cocycle is

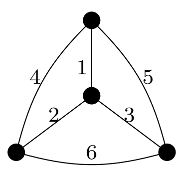


Figure 1: The cocycle in degree 3.

given by the 3-wheel as seen in Figure 1 and the corresponding $\mathfrak{grt}_1$ element is then

$$\sigma_3 := -24[X,[X,Y]] + 24[[X,Y],Y]$$

For the 5 and 7 cocycle the results can be found in Appendix A and B. Importantly this gives explicit descriptions of generators of $\mathfrak{grt}_1$ in degree 3, 5 and 7.

Finally, we can combine the calculation of the coefficients $c_{2n}, c_{\alpha,\beta}, c_{\alpha,\beta,\gamma}$ and the map ϕ to completely calculate τ_3, τ_5 and τ_7 as well as give concise descriptions of τ_9, τ_{11} and τ_{13} (up to depth 3). They are given as follows:

$$\begin{aligned}
\tau_3 &= -\frac{5}{2}\cdot\sigma_3\frac{\zeta(3)}{(2\pi i)^3} = 60\frac{\zeta(3)}{(2\pi i)^3}\left([X,[X,Y]] - [[X,Y],Y]\right)\\
\tau_5 &= 126\cdot\sigma_5\frac{\zeta(5)}{(2\pi i)^5} = 630\frac{\zeta(5)}{(2\pi i)^5}(-2\cdot[Y,[Y,[Y,[Y,X]]]] + 4\cdot[Y,[Y,[[Y,X],X]]]\\
&\qquad\qquad - 3\cdot[[Y,[Y,X]],[Y,X]] - 4\cdot[Y,[[[Y,X],X],X]]\\
&\qquad\qquad - [[Y,X],[[Y,X],X]] + 2\cdot[[[[Y,X],X],X],X])\\
\tau_7 &= -1716\cdot\sigma_7\frac{\zeta(7)}{(2\pi i)^7}\\
\tau_9 &= 437580\cdot\sigma_9\frac{\zeta(9)}{(2\pi i)^9}\\
\tau_{11} &= \frac{\zeta(11)}{(2\pi i)^{11}}\cdot(7759752\cdot\sigma_{11}) + \left(\frac{\zeta_{\mathrm{sv}}(5,3,3)}{(2\pi i)^{11}} + \frac{22020}{3553}\frac{\zeta(3)^2\zeta(5)}{(2\pi i)^{11}}\right)\left(-\frac{323323}{2400}\cdot[\sigma_3,[\sigma_3,\sigma_5]_{\mathrm{Ih}}]_{\mathrm{Ih}}\right)
\end{aligned}$$

and

$$\begin{aligned}
\tau_{13} &= \frac{\zeta(13)}{(2\pi i)^{13}}\cdot(135207800\cdot\sigma_{13})\\
&+ \left(\frac{\zeta_{\mathrm{sv}}(7,3,3)}{(2\pi i)^{13}} - \frac{244740}{5681}\frac{\zeta(5)^2\zeta(3)}{(2\pi i)^{13}} + \frac{123508}{7429}\frac{\zeta(7)\zeta(3)^2}{(2\pi i)^{13}}\right)\left(\frac{2414425}{4032}\cdot[\sigma_3,[\sigma_3,\sigma_7]_{\mathrm{Ih}}]_{\mathrm{Ih}}\right)\\
&+ \left(\frac{\zeta_{\mathrm{sv}}(5,5,3)}{(2\pi i)^{13}} - \frac{203950}{5681}\frac{\zeta(5)^2\zeta(3)}{(2\pi i)^{13}}\right)\left(-\frac{676039}{600}\cdot[\sigma_5,[\sigma_5,\sigma_3]_{\mathrm{Ih}}]_{\mathrm{Ih}} - \frac{482885}{672}\cdot[\sigma_3,[\sigma_3,\sigma_7]_{\mathrm{Ih}}]_{\mathrm{Ih}}\right)
\end{aligned}$$

where $\sigma_i \in \mathfrak{grt}_1$ and σ_3 is defined as above, σ_5 and σ_7 are defined in Appendix A and B and σ_9, σ_{11} and σ_{13} are defined up to depth 3 in Section 4.6.

Before proceeding, we would like to highlight two interesting aspects of further study. On one hand, our calculation of the coefficient c_Γ of the wheel graph shows that single-valued integration is well-suited for computing the integrals in the definition of c_Γ. Moreover, it can produce closed form results for infinite families. A natural next step would be to extend the results to other graphs. This, combined with with the implementation of the map $\phi : \mathsf{GC} \to \mathfrak{sder}_2$, would give more information about elements of $\mathfrak{grt}_1$ as well as graph cocycles in GC.

On the other hand, in [3] Brown defined another kind of integrals for graphs in GC. These, so called canonical integrals, are defined via invariant differential forms and their evaluation can, in principle, give much more complicated transcendental numbers than multiple zeta values. However, if we compare our value c_Γ of the $2n+1$-wheel from Theorem 2.16 with the conjectured value of the canonical integral of the $2n+1$-wheel

$$I_{W_{2n+1}}(\omega^{4n+1}) \overset{?}{=} 2(4n+1)\binom{4n}{2n}\zeta(2n+1)$$

we notice that they are equal (up to the $(2\pi i)^{2n+1}$ factor). This leads to the following conjecture:

Conjecture 1.2. *The integrals c_Γ for graphs on $2n$ vertices are equal to the canonical integrals of the invariant differential form ω^{4n+1} as defined in [3].*

If one now succeeds in calculating more coefficients c_Γ of graphs in GC this could give further insights into the connection between c_Γ and the canonical integrals.

Notation, conventions and binomial Identities

We denote by $\mathbb{N}$ the natural numbers $\{1, 2, 3, \ldots\}$ and by $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. Further δ_{ij} is the Kronecker delta i.e. $\delta_{ij} = 1$ if $i = j$ and 0 else. Moreover, the symmetric groups will be denoted by $\mathbb{S}_n$ and an element of $\mathbb{S}_n$ which would normally be written in cycle notation as $(i_1 i_2 \ldots i_k)$ will be denoted by $(i_1; i_2; \ldots; i_k)$.

We write $\mathbb{F}_{\text{Lie}}$ for the free Lie algebra in two generators and $\mathbb{F}_{\text{Lie}}(x, y)_n$ the subspace spanned by Lie words with $n-1$ brackets. Then we denote the completed free Lie algebra in two generators by

$$\widehat{\mathbb{F}}_{\text{Lie}}(x, y) := \prod_{n \geq 1} \mathbb{F}_{\text{Lie}}(x, y)_n.$$

Moreover, its topological universal enveloping algebra is $\mathbb{K}\langle\langle x, y\rangle\rangle$ that is the space of formal power series in the non-commuting variables x and y.

We also follow classical conventions for binomial coefficients that is $\binom{n}{k} = 0$ if $k > n$ or $k < 0$. Furthermore, over the course of this work we are often going to need and refer to the following classical binomial identities:

Lemma 1.3. *The following identities hold:*

1. *Let* $\overline{n}, \overline{k} \in \mathbb{N}_0$ *then*

$$\binom{\overline{n}}{\overline{h}}\binom{\overline{n}-\overline{h}}{\overline{k}} = \binom{\overline{n}}{\overline{k}}\binom{\overline{n}-\overline{k}}{\overline{h}} = \binom{\overline{n}}{\overline{h}+\overline{k}}\binom{\overline{h}+\overline{k}}{\overline{h}}.$$

2. *Let* $\overline{m}, \overline{r}, \overline{s}, \overline{t} \in \mathbb{N}_0$ *then*

$$\sum_{\overline{k}=0}^{\overline{r}} \binom{\overline{r}-\overline{k}}{\overline{m}}\binom{\overline{s}}{\overline{k}-\overline{t}}(-1)^{\overline{k}-\overline{t}} = \binom{\overline{r}-\overline{t}-\overline{s}}{\overline{r}-\overline{t}-\overline{m}}.$$

3. *Let* $\overline{n} \in \mathbb{N}_0$ *then*

$$\sum_{\overline{j}=0}^{\overline{n}} (-1)^{\overline{j}}\binom{\overline{n}}{\overline{j}} = 0.$$

4. *Let* $\overline{n} \geq \overline{k} \geq 0$*. Then the Hockey-stick identity is*

$$\sum_{\overline{m}=\overline{k}}^{\overline{n}} \binom{\overline{m}}{\overline{k}} = \binom{\overline{n}+1}{\overline{k}+1}.$$

5. *Let* $\overline{r} \geq 1$ *and* $\overline{k} \geq 0$*. Then*

$$\binom{-\overline{r}}{\overline{k}} = (-1)^{\overline{k}}\binom{\overline{r}+\overline{k}+1}{\overline{k}}.$$

6. *Let* $\overline{m}, \overline{n}, \overline{r}, \overline{s} \in \mathbb{N}_0$ *such that* $\overline{n} \geq \overline{s}$*. Then*

$$\sum_{\overline{k}=0}^{\overline{r}} \binom{\overline{r}-\overline{k}}{\overline{m}}\binom{\overline{s}+\overline{k}}{\overline{n}} = \binom{\overline{r}+\overline{s}+1}{\overline{m}+\overline{n}+1}.$$

We acknowledge that this notation with the $^{-}$ is rather ugly. However, it is needed to distinguish these variables from the often similarly named variables appearing in the proofs. With this out of the way we can start by introducing multiple zeta values.

2 Prerequisites

2.1 Multiple zeta values

In this section we mostly follow [12] and [4]. The multiple zeta functions are a generalisation of the Riemann zeta function and are defined as follows:

Definition 2.1. Let $k \in \mathbb{N}$, $n_1 \geq 2$ and $n_i \geq 1$ for $i \in \{2, \ldots, k\}$. Then the multiple zeta functions are given by

$$\zeta(n_1, \ldots, n_k) := \sum_{j_1 > j_2 > \ldots > j_k \geq 1} \frac{1}{j_1^{n_1} j_2^{n_2} \ldots j_k^{n_k}}$$

and we call a value $\zeta(n_1, \ldots, n_k)$ a *multiple zeta value* (MZV). For $k = 1$ this reduces to the Riemann zeta function.

Let $\mathcal{Z}$ denote the $\mathbb{Q}$-algebra spanned by all multiple zeta values over $\mathbb{Q}$. Let further $\mathcal{Z}_N$ denote the $\mathbb{Q}$-vector space spanned by the MZVs of total weight $N = n_1 + \ldots + n_r$. Then $\mathcal{Z}$ is the sum of the vector spaces $\mathcal{Z}_N$.

We can extend this definition of MZVs to words w in x, y. We say that a word w is *admissible* if it starts with an x and ends in a y. For such words $w = x^{n_1} y x^{n_2} y \ldots x^{n_k} y$ for $n_1 \geq 2$ and $n_i \geq 1$ for $i > 1$ we define

$$\zeta(w) = \zeta(n_1 + 1, \ldots, n_k + 1).$$

Moreover, we define $\zeta(\varnothing) := 1$ where $\varnothing$ denotes the empty word. Further, let B be the $\mathbb{Q}$-vector space of words in x, y and let $B_{\mathrm{adm}} \subseteq B$ be the subspace of admissible words. By linearity the above definition can be extended to B. On B the following product can be defined:

Definition 2.2. Let $w, w' \in B$ and $\alpha, \alpha' \in \{x, y\}$ a letter. Then we define the *shuffle product* $⧢$ of αw and $\alpha' w'$ recursively by

$$\alpha w ⧢ \alpha' w' = \alpha(w ⧢ \alpha' w') + \alpha'(\alpha w ⧢ w'),$$

and $w ⧢ 1 = 1 ⧢ w = w$.

The shuffle product is associative and commutative and corresponds to the sum of all possibilities of interlacing the two words. Moreover, the map $\zeta : (B_{adm}, ⧢) \to \mathbb{R}$ is a homomorphism of commutative algebras and extends uniquely to a morphism of algebras $\zeta : (B, ⧢) \to \mathbb{R}$ such that $\zeta(x) = \zeta(y) = 0$. The MZVs obtained like this, for non-admissible words, are being called *shuffle regularized multiple zeta values.* The process of regularization is described by the following lemma for $n_1 \geq 1$:

Lemma 2.3. *Let $w = x^{n_1} y x^{n_2} y \ldots x^{n_{r-1}} y x^{n_r}$ with $n_1 \geq 1$ then*

$$\zeta(w) = (-1)^{n_r} \sum_{\substack{k_i \geq n_i \\ \sum k_i = \sum n_i}} \prod_{i=i}^{r} \binom{k_i}{n_i} \zeta(k_1 + 1, \ldots, k_r + 1).$$

In particular, for the case of $r = 4$ we find for a word $w = x^a y x^b y x^c y x^d$ with $a \neq 0$

$$\zeta(w) = (-1)^d \sum_{0 \leq j+k \leq d} \binom{a+k}{a} \binom{b+j}{b} \binom{c+d-j-k}{c} \zeta(a+k+1, b+j+1, c+d-j-k+1)$$

and in the case of $r=3$ we find for $w = x^a y x^b y x^c$ with $a \neq 0$

$$\zeta(x^a y x^b y x^c) = (-1)^c \sum_{i=0}^{c} \binom{a+i}{a} \binom{b+c-i}{b} \zeta(a+i+1, b+c-i+1).$$

For a proof of this theorem see Lemma 2.3 in [19]. In the case of a word where n_1 is not ≥ 1 we can also apply the above formula to remove the x^{n_r} from the end. However, some terms of the form $\zeta(1, \ldots)$ will appear. These correspond to words $yx^{m_1}yx^{m_2}y \ldots yx^{m_{r-2}}y$. For these words we then apply the same idea as above, however now, to the y on the left. That is we expand the shuffle product $\zeta(y \sqcup\!\sqcup x^{m_1}y \ldots x^{m_{k-2}}y)$ and then use the fact that this equals 0 to deduce the formula. In the case that n_1 to n_i are all 0 this regularization with y needs to be applied repeatedly until for all terms of ζ the leading argument is unequal 1. This procedure is best demonstrated by an example:

Example 2.4. Consider the word y^3x. To compute $\zeta(y^3x)$ we need to apply shuffle regularization as explained above. We get

$$0 = \zeta(y^3 \sqcup\!\sqcup x) = \zeta(xy^3) + \zeta(yxy^2) + \zeta(y^2xy) + \zeta(y^3x)$$

and thus $\zeta(y^3x) = -\zeta(xy^3) - \zeta(yxy^2) - \zeta(y^2xy)$. The first term on the left after the equality is in admissible form and evaluates to $\zeta(2,1,1)$. The second and third term however still need more work. We compute

$$0 = \zeta(y \sqcup\!\sqcup xy^2) = \zeta(yxy^2) + 3 \cdot \zeta(xy^3) \Rightarrow \zeta(yxy^2) = -3 \cdot \zeta(xy^3)$$

as well as

$$0 = \zeta(y \sqcup\!\sqcup yxy) = 2\zeta(y^2xy) + 2\zeta(yxy^2) \Rightarrow \zeta(y^2xy) = -\zeta(yxy^2) = 3 \cdot \zeta(xy^3),$$

where in the second equality after the implication we used the result from the previous equation. This is necessary as $\zeta(yxy^2)$ is not in admissible form and therefore the procedure needs to be applied to it again. Finally, we get

$$\zeta(y^3x) = -\zeta(xy^3) + 3 \cdot \zeta(xy^3) - 3 \cdot \zeta(xy^3) = -\zeta(2,1,1).$$

The relations $\zeta(w)\zeta(w') = \zeta(w \sqcup\!\sqcup w')$ for $w, w' \in \{x,y\}^*$ are called *shuffle relations*. Apart from the shuffle relations there are two more types of relations between MZVs which we will now present.

Definition 2.5. Let $v_i = x^{i-1}y$. The *stuffle product* $\star : B \times B \to B$ is defined inductively by:

$$\begin{aligned} w \star 1 = 1 \star w = w \quad \text{for all} \quad w \in \{x,y\}^* \\ v_i w \star v_j w' = v_i(w \star v_j w') + v_j(v_i w \star w') + v_{i+j}(w \star w') \end{aligned}$$

for all $i, j \geq 1$ and $w, w' \in \{x,y\}^*$. The *stuffle relation* is then:

$$\zeta(w)\zeta(w') = \zeta(w \star w').$$

Intuitively, this product comes from the representation of MZVs as nested sums. For example it holds that

$$\sum_{k\geq 1} \frac{1}{k^m} \sum_{l \geq 1} \frac{1}{l^n} = \sum_{k<l} \frac{1}{k^m l^n} + \sum_{l<k} \frac{1}{k^m l^n} + \sum_{k=l} \frac{1}{k^m l^n}$$

from which the following relation for MZVs follows $\zeta(m)\zeta(n) = \zeta(n,m) + \zeta(m,n) + \zeta(m+n)$.

Lastly, we have the *regularization* relation. Let $w \in B_{\text{adm}}$, then it can be shown that $y \star w - y \sqcup\!\sqcup w \in B_{\text{adm}}$ is also a linear combination of admissible words. The regularization relation (or Hoffman relation) is then given by

$$\zeta(y \star w - y \sqcup\!\sqcup w) = 0.$$

This is best illustrated by a simple example:

Example 2.6. Let $w = xy$. Then we have

$$y \star xy = v_1 \star v_2 = v_1(1 \star v_2) + v_2(v_1 \star 1) + v_3(1 \star 1) = yxy + xyy + xxy$$

as well as $y \sqcup\!\sqcup xy = yxy + 2xyy$. The regularization relation is then

$$\zeta(y \star xy - y \sqcup\!\sqcup xy) = \zeta(xxy + xyy) = 0$$

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

Further, for odd MZVs of depth two and odd weight by applying the above described relations the following parity theorem can be shown:

Theorem 2.7. *The double zeta value $\zeta(n,m)$ $(n \geq 1,\ m \geq 2)$ of weight $n+m = k = 2K+1$ is given in terms of products $\zeta(2s)\zeta(k-2s)$ $(0 \leq s \leq K-1)$ by*

$$\zeta(n,m) = (-1)^m \sum_{s=0}^{K-1} \left[\binom{k-2s-1}{m-1} + \binom{k-2s-1}{n-1} - \delta_{n,2s} + (-1)^m \delta_{s,0} \right] \zeta(2s)\zeta(k-2s).$$

A proof of this theorem can be found in [23, Section 5, Prop. 7].

It is conjectured that all algebraic relations over $\mathbb{Q}$ satisfied by the multiple zeta values are generated by the three types of relations given above (shuffle, stuffle, regularization). A conjectured minimal basis of the MZVs for small weights is then given as in the table below.

Weight	1	2	3	4	5	6	7	8
		$\zeta(2)$	$\zeta(3)$	$\zeta(4)$	$\zeta(5)$ $\zeta(2)\zeta(3)$	$\zeta(6)$ $\zeta(3)^2$	$\zeta(7)$ $\zeta(2)\zeta(5)$ $\zeta(3)\zeta(4)$	$\zeta(8)$ $\zeta(3)\zeta(5)$ $\zeta(3)^2\zeta(2)$ $\zeta(5,3)$

Notice that up to weight 7 only single zetas appear. Then in weight 8 a new irreducible quantity $\zeta(5,3)$ appears. There are multiple conjectures on the dimension of the vector space spanned by the $\zeta(w) \in \mathbb{R}$. This is best summarized by the reformulation in a specific Hopf algebra. Let $\mathcal{L}$ denote the free Lie algebra generated by one element σ_{2n+1} in every odd degree $-2n-1$ for $n \geq 1$ and no generators in the even degrees. Then, in decreasing weight, the underlying vector space is generated by

$$\sigma_3, \sigma_5, \sigma_7, [\sigma_5, \sigma_3], \sigma_9, [\sigma_7, \sigma_3], \sigma_{11}, [\sigma_3, [\sigma_3, \sigma_5]], \ldots.$$

Let $\mathbb{M}'$ be the graded dual of the universal enveloping algebra of $\mathcal{L}$, that is $\mathbb{M}'$ is the set of all non-commutative words in f_{2n+1} in degree $2n+1$ such that f_{2n+1} are dual to σ_{2n+1} equipped with the shuffle product. Let f_2 be a new generator in degree 2 which commutes with all the other generators and define

$$\mathbb{M} = \mathbb{Q}[f_2] \otimes_{\mathbb{Q}} (\mathbb{Q}\langle f_3, f_5, f_7, \ldots \rangle, \sqcup\!\sqcup).$$

The generators in each weight then match exactly with the table of MZVs above. Goncharov's conjecture from [14] is then:

Conjecture 2.8. *The algebra spanned by the multiple zeta values over $\mathbb{Q}$ is isomorphic to $\mathbb{M}$.*

This for example implies, as $\mathbb{M}$ is graded by weight, that no algebraic relations between MZVs of different weights should exist. On a side note, in [5] Brown introduced the motivic multiple zeta values, that are period integrals over a specific pro-algebraic variety. For these the above conjecture is a known theorem and motivic MZVs are a helpful tool to better understand the relations between MZVs. To continue our exposition of MZVs we first need to digress and introduce multiple polylogarithms and explain their connection to the MZVs. Then we are in a place to define a subset of the MZVs known as single-valued multiple zeta values.

2.2 Polylogarithms

In this section we closely follow [4]. Let M be a smooth manifold and $\gamma : [0,1] \to M$ a smooth curve on M. For smooth 1-forms ω_i on M we denote the pullback $\gamma^*(\omega_i)$ by $f_i(t)\,\mathrm{d}t$. Analogously to the definition of a line integral on M we have:

Definition 2.9. The *iterated integral* of $\omega_1, \ldots, \omega_n$ along γ is defined by

$$\int_\gamma \omega_1 \ldots \omega_n = \int_{0 \le t_1 \le \ldots \le t_n \le 1} f_1(t_1) \ldots f_n(t_n)\,\mathrm{d}t_1 \ldots \mathrm{d}t_n \,.$$

We can extend this definition by linearity and define the empty iterated integral ($n = 0$) to be the constant function 1.

The following properties hold for iterated integrals:

Proposition 2.10.
1. *The iterated integral $\int_\gamma \omega_1 \ldots \omega_n$ is invariant under reparametrization of γ.*
2. *Let $\gamma^{-1}(t)$ denote the inverse path $\gamma(1-t)$ of γ then*

$$\int_{\gamma^{-1}} \omega_1 \ldots \omega_n = (-1)^n \int_\gamma \omega_n \ldots \omega_1.$$

3. *If $\alpha, \beta : I \to M$ are two paths such that $\beta(0) = \alpha(1)$ and $\alpha\beta$ denotes the path obtained by first traversing α and then β. Then the iterated integral along $\alpha\beta$ can be expressed as*

$$\int_{\alpha\beta} \omega_1 \ldots \omega_n = \sum_{i=0}^{n} \int_\alpha \omega_1 \ldots \omega_i \int_\beta \omega_{i+1} \ldots \omega_n.$$

4. *There is the shuffle product formula*

$$\int_\gamma \omega_1 \ldots \omega_r \int_\gamma \omega_{r+1} \ldots \omega_{r+s} = \sum_{\sigma \in \Sigma(r,s)} \int_\gamma \omega_{\sigma(1)} \ldots \omega_{\sigma(r+s)},$$

where $\Sigma(r,s)$ denotes the set of (r,s)-shuffles:

$$\Sigma(r,s) = \{\sigma \in \Sigma(r+s) \mid \sigma^{-1}(1) < \ldots < \sigma^{-1}(r) \text{ and } \sigma^{-1}(r+1) < \ldots < \sigma^{-1}(r+s)\}$$

that is all ways to interlace the sequences $1, \ldots, r$ and $r+1, \ldots, r+s$ and $\Sigma(n)$ is the set of all permutations of $\{1, \ldots, n\}$.

Classically, polylogarithms have been defined as the series

$$\mathrm{Li}_n(z) := \sum_{k=1}^{\infty} \frac{z^k}{k^n}$$

for $n \geq 1$ which converges for $|z| < 1$ and thus defines a holomorphic function around the origin. The polylogarithms are a generalization of $\mathrm{Li}_1(z) = -\log(1-z)$ and satisfy the differential equations

$$\frac{\mathrm{d}}{\mathrm{d}z} \mathrm{Li}_n(z) = \frac{1}{z} \mathrm{Li}_{n-1}(z)$$

for $n \geq 2$. Solving this differential equation we find that they can also be defined by

$$\mathrm{Li}_n(z) = \int_\gamma \frac{1}{t} \mathrm{Li}_{n-1}(t)\, \mathrm{d}t$$

where γ is a smooth path from 0 to z in $\mathbb{C} \setminus \{0,1\}$. This shows that the polylogarithms have an analytic continuation to a multivalued function on $\mathbb{C} \setminus \{0,1\}$. Let us define the following 1-forms

$$\omega_0 = \frac{\mathrm{d}z}{z} \qquad \omega_1 = \frac{\mathrm{d}z}{z-1}.$$

Then by solving the recursion in the integral definition of $\mathrm{Li}_n(z)$ we find that

$$\mathrm{Li}_n(z) = -\int_\gamma \underbrace{\omega_0 \dots \omega_0}_{n-1} \omega_1 = -\int_{1 \geq t_1 \geq \dots \geq t_n \geq 0} \frac{\mathrm{d}t_1}{t_1} \cdots \frac{\mathrm{d}t_{n-1}}{t_{n-1}} \frac{z\, \mathrm{d}t_n}{zt_n - 1}.$$

This definition of polylogarithms can be extended to multiple polylogarithms:

Definition 2.11. Let $n_1, \dots, n_r \in \mathbb{N}$. Then the *multiple polylogarithms in one vairable* are defined by

$$\mathrm{Li}_{n_1,\dots,n_r}(z) = \sum_{k_1 > \dots > k_r \geq 1} \frac{z^{k_r}}{k_1^{n_1} \dots k_r^{n_r}}.$$

These are often also referred to as *hyperlogarithms*.

Similarly to the case of classical polylogarithms, one finds that

$$\frac{\mathrm{d}}{\mathrm{d}z} \mathrm{Li}_{n_1,\dots,n_r}(z) = \begin{cases} \frac{1}{z} \mathrm{Li}_{n_1,\dots,n_r - 1}(z) & \text{for } n_r > 1 \\ \frac{1}{z-1} \mathrm{Li}_{n_1,\dots,n_{r-1}}(z) & \text{for } n_r = 1. \end{cases}$$

as well as that the multiple polylogarithms can be written as iterated integrals

$$\mathrm{Li}_{n_1,\dots,n_r}(z) = (-1)^r \int_\gamma \omega_0^{n_1 - 1} \omega_1 \dots \omega_0^{n_r - 1} \omega_1$$

where again γ is a smooth path in $\mathbb{C} \setminus \{0,1\}$ from 0 to z. This defines an analytic continuation of $\mathrm{Li}_{n_1,\dots,n_r}$ on $\mathbb{C} \setminus \{0,1\}$. Finally, notice that all these integrals end with ω_1. Therefore, it is natural to define the integrals ending with ω_0. This can be done more generally by considering again the vector space B of words in x, y over $\mathbb{Q}$. Then for a word $w = x^{n_1 - 1} y \dots x^{n_r - 1} y$ we let

$$\mathrm{Li}_w(z) = (-1)^r \int_0^z \omega_0^{n_1 - 1} \omega_1 \dots \omega^{n_r - 1} \omega_1.$$

and extend this definition by linearity over words. By the shuffle product formula for iterated integrals we have

$$\mathrm{Li}_u(z)\, \mathrm{Li}_v(z) = \mathrm{Li}_{u ⧢ v}(z).$$

Finally, as every word in B can be written as a unique sum of shuffles

$$w = \sum_{i=0}^{k} w_i \sqcup\!\sqcup\, x^i.$$

where $w_i \in B_{\text{adm}}$ we can extend this definition of Li_w to all words $w \in B$ by setting

$$\text{Li}_{x^n}(z) = \int_\gamma \underbrace{\omega_0 \dots \omega_0}_{n} = \frac{1}{n!} \log^n(z)$$

and then defining $\text{Li}_w(z) = \sum_{i=0}^{k} \text{Li}_{w_i}(z) \, \text{Li}_{x^i}(z)$. With this definition the multiple polylogarithms can be described as the unique solution to the differential equations

$$\mathrm{d}\, \text{Li}_{w0}(z) = \omega_0 \, \text{Li}_w(z) \quad \text{and} \quad \mathrm{d}\, \text{Li}_{w1}(z) = \omega_1 \, \text{Li}_w(z)$$

with the constraints $\lim_{z \to 0} \text{Li}_w(z) = 0$ for all words $w \neq x^n$ and $\text{Li}_{x^n}(z) = \frac{1}{n!} \log^n(z)$. We can also consider the generating series of the $\text{Li}_w(z)$:

$$L(z) := \sum_{w \in \{x,y\}^*} \frac{\text{Li}_w(z)}{(2\pi i)^{|w|}} w.$$

That is $L(z)$ defines a multivalued function on M taking values in $\mathbb{C}\langle\langle x, y \rangle\rangle$ and satisfies the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}z} L(z) = \frac{1}{2\pi i} \left(\frac{x}{z} + \frac{y}{z-1} \right) L(z).$$

This equation is also known as the Knizhnik-Zamolodchikov equation (short KZ-equation). The above constraints can then be written as $L(z) \sim \exp(x \log(z))$ as $z \to 0$, this means that there exists a $\mathbb{C}\langle\langle x, y \rangle\rangle$-valued function $h(z)$, holomorphic around the origin, such that $L(z) = h(z) \exp(x \log(z))$ for z near 0 and $h(0) = 1$. This condition uniquely determines the solution $L(z)$ to the KZ-equation. Similarly, one finds another solution $L^1(z)$ to the KZ-equation satisfying

$$L^1(z) \sim \exp(y \log(1-z)) \quad \text{as} \quad z \to 1.$$

This series has leading term 1 and is thus invertible. It is custom to then consider the parallel transport:

$$\Phi(z) = (L^1(z))^{-1} L(z).$$

From differentiating $L^1(z)\Phi(z) = L(z)$ one finds that $\mathrm{d}\Phi(z) = 0$ and thus $\Phi(z)$ is a constant series denoted by $\Phi_{KZ}(x, y) \in \mathbb{C}\langle\langle x, y \rangle\rangle$ called the KZ-associator. This series is a Drinfel'd associator as defined in Section 2.5 and we will come back to it there. For now notice that this series can be written as

$$\Phi_{KZ}(x, y) = \lim_{z \to 1^-} \exp(-y \log(1-z)) L(z).$$

From the constraint for $L^1(z)$ it follows that every multiple polylogarithm $\text{Li}_w(z)$ has a canonical branch for $z \in (0, 1)$, which can be written as

$$\text{Li}_w(z) = a_0(z) + a_1(z) \log(1-z) + \ldots + a_{|w|}(z) \log^{|w|}(1-z)$$

where $a_i(z)$ is holomorphic in a neighbourhood of 1. We can then define the regularized value at 1 as

$$\text{Reg}_{z=1} \text{Li}_w(z) = a_0(1),$$

and find that $\Phi_{KZ}(x, y)$ is the generating series of these regularized values (up to the $(2\pi i)^{|w|}$).

This leads us back to the multiple zeta values, notice that for all words $w \in B_{\text{adm}}$ the $\text{Li}_w(z)$ converge at the point $z = 1$ and we have $\zeta(w) = \text{Li}_w(z)$. One can then further show that for all words $w \in B$ it holds that

$$\zeta(w) = \text{Reg}_{z=1} \text{Li}_w(z),$$

and thus the multiple polylogarithms evaluated at 1 give an alternative definition of the MZVs. In particular the KZ-associator can be written as

$$\Phi_{KZ}(x, y) = \sum_{w \in \{x,y\}^*} \frac{\zeta(w)}{(2\pi i)^{|w|}} w.$$

2.3 Single-valued MZVs

In this section we mostly follow [7] and [6]. We can now turn to the definition of single-valued MZVs. For this consider again Φ_{KZ}. Then it was shown in [6] that there exists a unique element $y' \in \mathbb{C}\langle\langle x, y\rangle\rangle$ satisfying the fixed-point equation

$$\Phi_{KZ}(-x, -y')y'\Phi_{KZ}(-x, -y')^{-1} = \Phi_{KZ}(x, y)y\Phi_{KZ}(x, y)^{-1}.$$

The generating series for single-valued multiple polylogarithms can then be given by

$$\mathcal{L}(z) = \widetilde{L}_{-x,-y'}(\overline{z})^{-1} L_{x,y}(z).$$

where $\sim$ denotes the reversal of words. We define $\mathcal{L}_w(z)$ to be the coefficients of the expansion of the generating series

$$\mathcal{L}(z) = \sum_{w \in B} \frac{\mathcal{L}_w(z)}{(2\pi i)^{|w|}} w.$$

The $\mathcal{L}_w(z)$ are all single-valued functions of z, are linearly independent over $\mathbb{C}$, and satisfy the same shuffle relations and differential equations with respect to $\frac{\partial}{\partial z}$ as the $L_w(z)$. The value at 1 of the generating series is given by

$$\mathcal{L}(1) = \Phi_{KZ}(-x, -y')^{-1}\Phi_{KZ}(x, y).$$

The single-valued multiple zeta values $\zeta_{\text{sv}}(w)$ are then defined as the coefficients of this series

$$\Phi_{KZ}^{\text{sv}} := \mathcal{L}(1) = \sum_{w \in B} \frac{\zeta_{\text{sv}}(w)}{(2\pi i)^{|w|}} w$$

which we also call the *single-valued KZ-associator* as it can also be obtained from Φ_{KZ} by replacing every $\zeta(w)$ by its single-valued counterpart $\zeta_{\text{sv}}(w)$. Let us denote by $\mathcal{Z}^{\text{sv}} \subseteq \mathcal{Z}$ the subalgebra of $\mathcal{Z}$ spanned by the $\zeta_{\text{sv}}(w)$. The single-valued MZVs satisfy the same double shuffle and associator relations as usual MZVs and many more: For example we have that $\zeta_{\text{sv}}(2) = 0$ (and thus also $\zeta_{\text{sv}}(2n) = 0$ for all $n \geq 1$) as well as

$$\begin{aligned}
\zeta_{\text{sv}}(2n+1) &= 2\zeta(2n+1) \quad \text{ for all } n \geq 1 \\
\zeta_{\text{sv}}(3,5) &= 14\zeta(3)\zeta(5) \\
\zeta_{\text{sv}}(5,3,3) &= 2\zeta(5,3,3) - 5\zeta(3)^2\zeta(5) \\
\zeta_{\text{sv}}(5,5,3) &= 2\zeta(5,5,3) + 50\zeta(3)\zeta(5)^2 + 10\zeta(5,3)\zeta(5) \\
\zeta_{\text{sv}}(7,3,3) &= 2\zeta(7,3,3) - 14\zeta(3)^2\zeta(7) + 60\zeta(3)\zeta(5)^2 + 12\zeta(5,3)\zeta(5)
\end{aligned}$$

Remark 2.12. Later we are also going to need the following expansion of $\mathcal{L}_w(z)$ for words $w =$

0^n10^m in terms of Li's:

$$\mathcal{L}_{0^n10^m} = \sum_{k=0}^{n}(-1)^{k+1}\binom{m+k}{m}\frac{\ln(z\overline{z})^{n-k}}{(n-k)!}\,\mathrm{Li}_{m+k+1}(z)$$
$$+\sum_{k=0}^{m}(-1)^{k+1}\binom{n+k}{n}\frac{\ln(z\overline{z})^{m-k}}{(m-k)!}\,\mathrm{Li}_{n+k+1}(z)$$

which was shown in [19, Example 2.10]. From this we deduce that $\mathcal{L}_{0^n10^m}(z) = \mathcal{L}_{0^m10^n}(\overline{z})$ for $n, m \in \mathbb{N}_0$.

In [7] Brown also gives algebra generators of $\mathcal{Z}^{\mathrm{sv}}$ for small weights:

N	3	5	7	9	11	13
Generators of $\mathcal{Z}^{\mathrm{sv}}$	$\zeta_{\mathrm{sv}}(3)$	$\zeta_{\mathrm{sv}}(5)$	$\zeta_{\mathrm{sv}}(7)$	$\zeta_{\mathrm{sv}}(9)$	$\zeta_{\mathrm{sv}}(11)$ $\zeta_{\mathrm{sv}}(5,3,3)$	$\zeta_{\mathrm{sv}}(13)$ $\zeta_{\mathrm{sv}}(5,5,3)$ $\zeta_{\mathrm{sv}}(7,3,3)$

Remember now the Hopf algebra $\mathbb{M}$ from the end of Section 2.1. Let $\mathcal{U} := \mathbb{Q}\langle f_3, f_5, f_7, \ldots\rangle$. Then there is a map $\mathrm{sv} : \mathbb{M} \to \mathcal{U}$ that sends $\mathrm{sv}(w) = 0$ for all $w \in \mathbb{M}$ such that f_2 is a letter in w and

$$\mathrm{sv}(w) = \sum_{uv=w} u \sqcup\!\sqcup\, \widetilde{v}$$

for every other $w \in \mathcal{U}$ where $\widetilde{\ }$ denotes the reversal of words and extend this by linearity. One can then show that $\mathrm{Im}(\mathrm{sv}) = \mathcal{Z}^{\mathrm{sv}}$. Thus, under the assumption that Conjecture 2.8 holds this gives a map from $\mathcal{Z} \to \mathcal{Z}^{\mathrm{sv}}$ which we will call the single-valued map. By way of example we have

$$\mathrm{sv}(f_a) = 2f_a, \quad \mathrm{sv}(f_af_b) = 2(f_af_b + f_bf_a)$$
$$\mathrm{sv}(f_af_bf_c) = 2(f_af_bf_c + f_af_cf_b + f_cf_af_b + f_cf_bf_a)$$

with odd $a, b, c \geq 3$. In general sv can be computed via the recursion

$$\mathrm{sv}(f_awf_b) = f_a\,\mathrm{sv}(wf_b) + f_b\,\mathrm{sv}(f_aw)$$

for $w \in \{f_{2n+1}\}^*$. From this, the above described relations between the single-valued MZVs can easily be calculated. Coming back to the definition of $\mathcal{L}(z)$ Brown showed in [7] that $y' = \psi y \psi^{-1}$ and thus that

Theorem 2.13.

$$\Phi_{KZ}^{\mathrm{sv}} = \mathcal{L}(1) = \psi$$

As an example we are interested in computing $\zeta_{\mathrm{sv}}(w)$ for words of depth 2. For odd length words we have:

Theorem 2.14. *Let $w = x^ayx^byx^c$ be a word of depth 2 of odd length $|w| = 2n+1$. Then we have that*

$$\frac{\zeta_{\mathrm{sv}}(w)}{(2\pi i)^{|w|}} = \left((-1)^{a+1}\binom{2n}{a} + (-1)^b\binom{2n}{b} + (-1)^{c+1}\binom{2n}{c}\right)\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}.$$

Proof. Let $2n+1$ be the length of w. First assume that $a \neq 0$. In this case we have

$$\begin{aligned}
\Phi_{KZ}(w) = \frac{\zeta(w)}{(2\pi i)^{2n+1}} &= (-1)^c \sum_{i=0}^{c} \binom{a+i}{a}\binom{b+c-i}{b} \frac{\zeta(a+i+1, b+c-i+1)}{(2\pi i)^{2n+1}} \\
&= (-1)^c \sum_{i=0}^{c}\sum_{s=0}^{n-1} \binom{a+i}{a}\binom{b+c-i}{b}(-1)^{b+c-i+1} \\
&\left(\binom{2n-2s}{b+c-i} + \binom{2n-2s}{a+i} - \delta_{a+i+1,2s} + (-1)^{b+c-i+1}\delta_{s,0}\right) \frac{\zeta(2s)\zeta(2n-2s+1)}{(2\pi i)^{2n+1}}
\end{aligned}$$

where we used the shuffle regularization Lemma 2.3 in the first equality and the parity theorem 2.7 in the second equality. If we consider Φ^{sv}_{KZ} notice that for $s \neq 0$ the expression contains $\zeta(2s)$ and thus vanishes. Therefore, we find

$$\Phi^{\mathrm{sv}}_{KZ}(w) = \sum_{i=0}^{c} \binom{a+i}{a}\binom{b+c-i}{b}(-1)^{b-i}\Bigg(\underbrace{\binom{2n}{b+c-i}}_{(I)} + \underbrace{\binom{2n}{a+i}}_{(II)} + \underbrace{(-1)^{b+c-i+1}}_{(III)}\Bigg)\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}$$

where we used that $\zeta(0) = -\frac{1}{2}$ and $\zeta_{\mathrm{sv}}(2n+1) = 2\zeta(2n+1)$. Now we can consider the three parts $(I), (II), (III)$ of the sum separately. Moreover, in the following we are going to omit the term $\zeta(2n+1)/(2\pi i)^{2n+1}$. We find for (II):

$$\begin{aligned}
(-1)^b \sum_{i=0}^{c}(-1)^i \binom{a+i}{a}\binom{2n}{a+i}\binom{b+c-i}{b} &= (-1)^b \binom{2n}{a}\sum_{i=0}^{b+c}\binom{2n-a}{i}\binom{b+c-i}{b} \\
&= (-1)^b\binom{2n}{a}\binom{-1}{c} = (-1)^{a+1}\binom{2n}{a}
\end{aligned}$$

where in the first equality we used the first identity from Lemma 1.3 with $\overline{n} = 2n, \overline{k} = i$ and $\overline{h} = a$ as well as that for $i > c$ the sum vanishes. In the second equality we used the second identity from Lemma 1.3 with $\overline{m} = b, \overline{k} = i, \overline{r} = b+c, \overline{s} = 2n-a$ and $\overline{t} = 0$. Finally, in the last equality we used the fifth identity from Lemma 1.3 as well as that $c + b = 2n - 1 - a$.

For (I) notice that by applying the substitution $i \mapsto c - j$ we get

$$(-1)^{a+1}\sum_{i=0}^{c}(-1)^i\binom{b+i}{b}\binom{2n}{b}\binom{a+c-i}{a} = (-1)^b\binom{2n}{b}$$

where we observed that the expression on the left is the same as the one for (I) (up to the sign) with a and b exchanged and thus we get the result on the right.

Finally for (III) we have:

$$(-1)^{c+1}\sum_{i=0}^{b}\binom{a+i}{a}\binom{b+c-i}{b} = (-1)^{c+1}\binom{a+b+c+1}{a+b+1} = (-1)^{c+1}\binom{2n}{c}$$

where we used the sixth identity from Lemma 1.3 with $\overline{b} = a, \overline{m} = a, \overline{r} = b+c, \overline{s} = a$ as well as that $a+b+c+1 = 2n$. Combining all the above this shows the result for the case of $a \neq 1$.

In the case of $a = 0$ we also apply shuffle regularization however one term will appear with the word $\zeta(yx^{b+c}y)$. This term then also needs to be shuffle regularized from the left by y and gives the second sum in the below expression. In total we have:

$$\Phi_{KZ}(w) = (-1)^c \sum_{i=1}^{c} \binom{0+i}{0}\binom{b+c-i}{b} \frac{\zeta(0+i+1, b+c-i+1)}{(2\pi i)^{2n+1}}$$
$$- (-1)^c \binom{b+c}{b} \left(\sum_{i=1}^{b+c} \frac{\zeta(i+1, b+c-i+1)}{(2\pi i)^{2n+1}} + \frac{\zeta(b+c+1, 1)}{(2\pi i)^{2n+1}} \right).$$

Notice that the first sum is the same as in the case of $a \neq 0$ with the only difference being the lower bound for i. We can thus consider Φ_{KZ}^{sv} and then replace this by the expression found above minus the terms corresponding to $i = 0$. This yields

$$\Phi_{KZ}^{\mathrm{sv}}(w) = \left((-1)^{0+1}\binom{2n}{0} + (-1)^b \binom{2n}{b} + (-1)^{c+1}\binom{2n}{c} \right) \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}$$
$$- (-1)^b \binom{b+c}{b} \Bigg(\underbrace{\binom{2n}{b+c}}_{(I)} + \underbrace{1 + (-1)^{b+c+1}}_{(II)} \Bigg) \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}$$
$$- (-1)^c \binom{b+c}{b} \underbrace{\sum_{i=1}^{b+c} \frac{\zeta_{\mathrm{sv}}(i+1, b+c-i+1)}{(2\pi i)^{2n+1}}}_{(III)} + \underbrace{\frac{\zeta_{\mathrm{sv}}(b+c+1, 1)}{(2\pi i)^{2n+1}}}_{(IV)}.$$

Let us first simplify the term (IV) by applying the parity theorem and using that $\zeta_{\mathrm{sv}}(2s) = 0$ for $s > 0$. We get:

$$(-1)^c \binom{b+c}{b} \frac{\zeta_{\mathrm{sv}}(b+c+1, 1)}{(2\pi i)^{2n+1}} = (-1)^c \binom{b+c}{b} \left(1 + \binom{2n}{b+c} - 1 \right) \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}.$$

which as $c = 2n-1-b$ cancels (I). Next let us investigate (III). Applying the parity theorem and once again noticing that only the terms for $s = 0$ contribute due to the single-valuedness we find for (III):

$$\begin{aligned}
&(-1)^c \binom{b+c}{b} \sum_{i=1}^{b+c} \frac{\zeta_{\mathrm{sv}}(i+1, b+c-i+1)}{(2\pi i)^{2n+1}} \\
&= (-1)^b \binom{b+c}{b} \sum_{i=1}^{b+c} (-1)^i \left(\binom{2n}{b+c-i} + \binom{2n}{i} + (-1)^{b+c-i+1} \right) \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}} \\
&= (-1)^b \binom{b+c}{b} \left(2n-1 + \sum_{i=1}^{2n-1} (-1)^i \binom{2n+1}{i+1} \right) \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}} \\
&= (-1)^b \binom{b+c}{b} \left(2n-1 - (-1)^{2n+1}\binom{2n+1}{2n+1} - \binom{2n+1}{2n} - \binom{2n+1}{0} \right) \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}} \\
&= 2 \cdot (-1)^{b+1} \binom{b+c}{b} \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}
\end{aligned}$$

where in the second equality we used that $b + c = 2n - 1$ as well as that $\binom{2n}{i+1} + \binom{2n}{i} = \binom{2n+1}{i+1}$. In the third equality we used the third identity from Lemma 1.3 and as the sum is not from 0 to $2n+1$ we got the three extra binomial coefficients. Now noticing that for (II) we have

$$(-1)^b \binom{b+c}{b} (1 + (-1)^{b+c+1}) \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}} = 2 \cdot (-1)^b \binom{b+c}{b} \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}$$

as $b+c+1=2n$, we see that (III) cancels with (II). Thus, what remains is

$$\frac{\zeta_{\mathrm{sv}}(w)}{(2\pi i)^{|w|}} = \left((-1)^{a+1}\binom{2n}{a} + (-1)^{b}\binom{2n}{b} + (-1)^{c+1}\binom{2n}{c}\right)\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}$$

for $a=0$ which proves the theorem. □

For even length words in depth 2 the parity theorem cannot be used. However, in Theorem 3.5 we describe a formula for calculating the depth 2 coefficients of ψ. From this and Theorem 2.13 a formula can easily be deducted:

Theorem 2.15. *Let $w = x^a y x^b y x^c$ be a word of depth 2 of even length $|w| = 2n$. Then we have*

$$\frac{\zeta_{\mathrm{sv}}(w)}{(2\pi i)^{|w|}} = 4\sum_{l+m=n-1}\left((-1)^{a+c}\binom{2l}{a}\binom{2m}{c} + (-1)^{a+b}\binom{2l}{b}\binom{2m}{a}\right.$$
$$\left. -(-1)^{b+c}\binom{2l}{b}\binom{2m}{c}\right)\frac{\zeta(2l+1)\zeta(2m+1)}{(2\pi i)^{2n}}.$$

In Proposition 3.7 we are also explicitly going to compute the depth 2 coefficients of ψ for odd length words thus showing Theorem 2.13 by example for the case of odd length depth 2 words.

2.4 Integrating the wheel graph

To apply the above introduced concepts of (single-valued) polylogarithms and MZVs we can now integrate the wheel graph as given in Figure 2 via equation (1) introduced by Rossi and Willwacher in [18] to obtain the corresponding coefficient in τ^t. For the definition of an order on the edges of a graph see Section 4. We denote by $|e|$ the order number of the edge e.

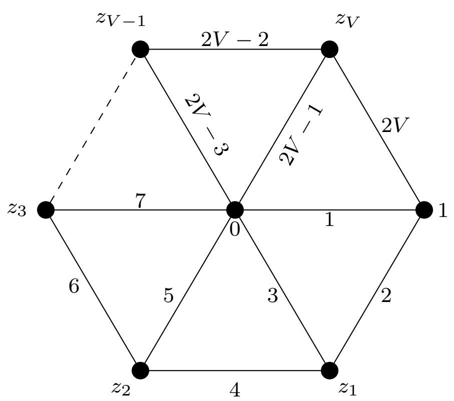


Figure 2: The V-wheel graph embedded into $\mathbb{C}$ fixed at 0 and 1

Theorem 2.16. *Let $V \in \mathbb{N}$ and denote by Γ the wheel graph on $V+1$ vertices as described in Figure 2. Then for even V, $c_\Gamma = 0$ and for $V = 2k+1$ odd it holds that*

$$c_\Gamma = 2(4k+1)\binom{4k}{2k}\frac{\zeta(2k+1)}{(2\pi i)^{2k+1}}.$$

Proof. Let $V \in \mathbb{N}$ denote the number of vertices of G minus 1 as in the theorem. We need to compute the integral from equation (1) for the wheel as shown in Figure 2. We can use the section of $\mathrm{Conf}_{V+1} \to C_{V+1}/S^1$ which identifies C_{V+1}/S^1 with $\mathrm{Conf}_{V-1}(\mathbb{C} \setminus \{0,1\})$ by fixing the first point of the configuration at $z_0 = 0$ and the second at $z_1 = 1$ for us this corresponds to the center vertex and the most right vertex respectively. Denote all other points by $z_2, \ldots, z_V$ corresponding to vertices as shown in Figure 2. Considering the integrand for the sum over edges e only the term with $e = (0,1)$ contributes, as we fixed the position of those two points. With this we find that $o(e, e') = (-1)^{e'-1}$.

Further let us denote by $w_x(z)$ the 1-form $\frac{\mathrm{d}z}{z-x}$ and let us call the edge e' the special edge. Since $\mathrm{Conf}_{V-1}(\mathbb{C} \setminus \{0,1\})$ is a complex manifold only terms with an equal number of holomorphic and antiholomorphic form components contribute (cf. [16], Section 6.6.1) and we can replace the $d\log$'s with $d\arg$'s. Moreover,

$$d\arg(|z-y|) = w_y(z) + w_z(y) - w_{\overline{y}}(\overline{z}) - w_{\overline{z}}(\overline{y}).$$

Then our expression reduces to

$$c_\Gamma = \frac{4^{V-1}}{2^{2V-2}} \int_{\mathbb{C}^V} \sum_{e' \neq (0,1)} (-1)^{e-1} \frac{1}{2\pi i} \log\left(\left|z_{s(e')} - z_{t(e')}\right|^2\right) \bigwedge_{e \in E \setminus \{e', (0,1)\}} \frac{1}{2\pi i} d\arg\left(\left|z_{s(e)} - z_{t(e)}\right|^2\right).$$

The idea of the integration is now as follows. We define two functions $f(k)$ and $\widetilde{f}(k)$. Here $f(k)$ describes the result of integrating out the first k vertices in the case that the special edge does not appear as any of those edges. That is, $f(0)$ is defined as the 1-form

$$f(0)(z_2) = d\arg(|z_2 - 1|^2) = w_1(z_2) - w_1(\overline{z_2})$$

and $f(k)$ can recursively be defined by

$$f(k)(z_{k+2}) = \frac{1}{2\pi i} \int_{z_{k+1}} f(k-1)(z_{k+1}) \wedge d\arg(|z_{k+1}|^2) \wedge d\arg(|z_{k+1} - z_{k+2}|^2)$$

where the integration domain is $\mathbb{C} \setminus \{0, 1, z_{k+2}\}$ with $z_{k+2} \neq 0, 1$. However, by standard arguments we can integrate over $\mathbb{C}$. This will be done throughout this proof and for the conciseness of the text not be mentioned anymore.

The function $\widetilde{f}(k)$ describes the result of integrating out the first $k-1$ vertices for all ways that the special edge e' can appear as an edge between those vertices. That is, $\widetilde{f}$ is recursively defined by

$$\widetilde{f}(1)(z_2) = -\log\left(|z_2 - 1|^2\right) = -\mathcal{L}_1(z_2)$$

and

$$\begin{aligned} \widetilde{f}(k)(z_{k+1}) = \frac{1}{2\pi i} \int_{z_k \in \mathbb{C}} & \widetilde{f}(k-1)(z_k) \wedge d\arg(|z_k|^2) \wedge d\arg(|z_k - z_{k+1}|^2) \\ & + \log\left(|z_k|^2\right) f(k-2)(z_k) \wedge d\arg(|z_k - z_{k+1}|^2) \\ & - \log\left(|z_k - z_{k+1}|^2\right) f(k-2)(z_k) \wedge d\arg(|z_k|^2), \end{aligned}$$

where the first term represents the case that the special edge already occurred before this vertex, the second term describes the situation where the special edge is the edge $(z_k, 0)$ and the final term describes the situation where the special edge is (z_k, z_{k+1}). We find the following two formulas for these functions:

Claim 2.17.

$$f(k)(z_{k+2}) = \mathcal{L}_{0^k}(z_{k+2})w_1(z_{k+2}) + (-1)^{k+1}\mathcal{L}_{0^k}(z_{k+2})w_1(\overline{z_{k+2}})$$
$$+ \sum_{n+m=k-1} \mathcal{L}_{0^n10^m}(z_{k+2})(-1)^{m+1}\left(\binom{k}{m}w_0(\overline{z_{k+2}}) + \binom{k}{n}w_0(z_{k+2})\right).$$

Claim 2.18.

$$\widetilde{f}(k)(z_{k+1}) = (2k-1)\sum_{n+m=k-1}(-1)^{m+1}\binom{k-1}{n}\mathcal{L}_{0^n10^m}(z_{k+1}).$$

Before we prove these claims we finish the main proof. Notice that the integrand can be expressed by

$$\frac{1}{(2\pi i)^V}\widetilde{f}(V)(1).$$

For even wheels i.e. V is even this is 0 as $\mathcal{L}(0^n10^m)(1) = \zeta_{\mathrm{sv}}(0^n10^m)$ which means that $\widetilde{f}(V)(1) = 0$ as only even single-valued zetas appear which are all 0. In the case of odd wheels i.e. $V = 2k+1$ for $k \in \mathbb{N}$ the expression is

$$(4k+1)\sum_{n+m=2k}(-1)^n\binom{2k}{n}\frac{\zeta_{\mathrm{sv}}(0^n10^m)}{(2\pi i)^{2k+1}} = (4k+1)\sum_{n=0}^{2k}\binom{2k}{n}^2\frac{\zeta_{\mathrm{sv}}(2k+1)}{(2\pi i^{2k+1}},$$

where we applied shuffle regularization. Using the special case of the Chu-Vandermonde identity $\sum_{j=0}^{m}\binom{m}{j}^2 = \binom{2m}{m}$ we find that this equals

$$(4k+1)\binom{4k}{2k}\frac{\zeta_{\mathrm{sv}}(2k+1)}{(2\pi i)^{2k+1}}$$

now from $\zeta_{\mathrm{sv}}(2k+1) = 2\zeta(2k+1)$ the result follows. ☐

Before we start with the proofs of the claims we are going to need the following identity:

Lemma 2.19. *Let $z, a, b \in \mathbb{C}$. Then*

$$d\log(z-a) \wedge d\log(z-b) = d\log\left(\frac{z-a}{z-b}\right) \wedge d\log(a-b).$$

Proof. First observe by partial fraction decomposition that

$$\frac{1}{(z-u)(z-v)} = \frac{1}{(z-u)(u-v)} + \frac{1}{(z-v)(v-u)}.$$

If we now expand the left side $d\log(z-a) \wedge d\log(z-b)$ we get

$$(w_a(z) + w_z(a)) \wedge (w_b(z) + w_z(b)) = w_a(z) \wedge w_z(b) + w_z(a) \wedge w_b(z) + w_z(a) \wedge w_z(b).$$

Now

$$w_a(z) \wedge w_z(b) = \frac{1}{(z-a)(b-z)}dz \wedge db = -\left(\frac{1}{(z-a)(a-b)} + \frac{1}{(z-b)(b-a)}\right)dz \wedge db$$
$$= w_a(z) \wedge w_a(b) - w_b(z) \wedge w_a(b) = (w_a(z) - w_b(z) - w_z(b)) \wedge w_a(b)$$

where in the second equality we used the observation from above and in the last equality we

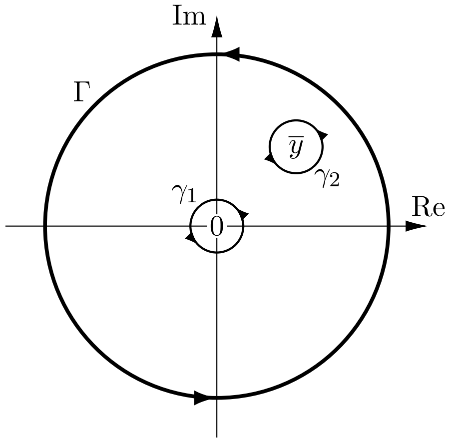


Figure 3: The boundary curve $\eta = \Gamma \cup \gamma_1 \cup \gamma_2$.

subtracted the vanishing term $w_z(b)$ on the left. Similarly, we find

$$w_z(a) \wedge w_b(z) = (w_a(z) + w_z(a) - w_b(z)) \wedge w_b(a)$$
$$w_z(a) \wedge w_z(b) = w_z(a) \wedge w_a(b) - w_z(b) \wedge w_b(a).$$

Adding up all the terms we get

$$(w_a(z) + w_z(a) - w_b(z) - w_z(b)) \wedge (w_a(b) + w_b(a)) = (d\log(z-a) - d\log(z-b)) \wedge d\log(a-b)$$

which shows the desired result. □

Proof of the first claim. We are going to proof the claim by induction. The base case of $k = 0$ follows trivially as we only get the contribution from the edge $(z_2, 1)$ which is given by

$$f(0) = w_1(z_2) - w_1(\overline{z_2}).$$

For the induction step assume the formula holds for k. Let us write $z := z_{k+1}$ and $y := z_{k+2}$. Let $w \in \{0,1\}^*$ containing at most one 1 and $a \in \{0,1\}$. Then

$$\frac{1}{2\pi i}\int_{z\in\mathbb{C}} \mathcal{L}_w(z) w_a(z) \wedge d\arg(|z|^2) \wedge d\arg(|z-y|^2)$$
$$= \frac{1}{2\pi i}\int_{z\in\mathbb{C}} \mathcal{L}_w(z)\left(\underbrace{w_a(z)\wedge w_0(\overline{z})\wedge w_{\overline{z}}(\overline{y})}_{(I)} + \underbrace{w_0(\overline{z})\wedge w_a(z)\wedge w_z(y)}_{(II)}\right).$$

Let us consider the first term (I). We apply Stokes' theorem as well as Lemma 2.19 to obtain

$$\frac{1}{2\pi i}\int_\eta \mathcal{L}_{wa}(z) w_0(\overline{z}) \wedge w_{\overline{z}}(\overline{y}) = \frac{1}{2\pi i}\int_\eta \mathcal{L}_{wa}(z)(w_0(\overline{z}) - w_{\overline{y}}(\overline{z})) \wedge w_0(\overline{y})$$

where we use the curve η as shown in Figure 3 consisting of Γ a circle of radius R and little circles of radius r cutting out the problematic points. Now:

$$\lim_{r\to 0}\frac{1}{2\pi i}\int_{\gamma_1} \mathcal{L}_{wa}(z) w_0(\overline{z}) \wedge w_0(\overline{y}) = \lim_{r\to 0}\frac{-1}{2\pi i}\int_0^{2\pi} \mathcal{L}_{wa}(re^{i\varphi})\frac{1}{re^{-i\varphi}}(-ire^{-i\varphi})d\varphi \wedge w_0(\overline{y})$$
$$= \mathcal{L}_{wa}(0) w_0(\overline{y}) = 0,$$

where we used the substitution to polar coordinates $\overline{z} = re^{-i\varphi}$ and the minus in front of the integral comes from the orientation. In the last equality we just used the fact that $\mathcal{L}_{wa}(0) = 0$. Similarly, we obtain

$$\lim_{r\to 0} \frac{1}{2\pi i} \int_{\gamma_2} -\mathcal{L}_{wa}(z) w_{\overline{y}}(\overline{z}) \wedge w_0(\overline{y}) = -\mathcal{L}_{wa}(y) w_0(\overline{y}).$$

As $r \to 0$ the first term $w_0(\overline{z})$ integrated around γ_2 and the second term $w_{\overline{y}}(\overline{z})$ integrated around γ_1 give 0; basically as $r\mathcal{L}_{wa}(r) \to 0$ as $r \to 0$. What remains is to calculate the integral around Γ as $R \to \infty$ which in a similar fashion as to above gives:

$$\begin{aligned}
\lim_{R\to\infty} \frac{1}{2\pi i} \int_{\Gamma} \mathcal{L}_{wa}(z)(w_0(\overline{z}) - w_{\overline{y}}(\overline{z})) \wedge w_0(\overline{y}) &= \lim_{R\to\infty} \frac{1}{2\pi i} \int_{\Gamma} -\mathcal{L}_{wa}(z) \frac{\overline{y}}{\overline{z}(\overline{z}-\overline{y})} d\overline{z} \wedge \omega_0(\overline{y}) \\
&= \lim_{R\to 0} \frac{1}{2\pi i} \int_{\Gamma} \mathcal{L}_{wa}\left(\frac{1}{w}\right) \frac{\overline{y}}{1-\overline{yw}} d\overline{w} \wedge w_0(\overline{y}) \\
&= \lim_{R\to 0} \frac{i}{2\pi i} \int_0^{2\pi} \mathcal{L}_{wa}\left(\frac{1}{Re^{i\varphi}}\right) \frac{Re^{-i\varphi}\overline{y}}{1-\overline{y}Re^{-i\varphi}} d\varphi \wedge w_0(\overline{y}) \\
&= 0,
\end{aligned}$$

where we used the substitution $\overline{z} \mapsto \frac{1}{\overline{w}}$ in the second equality and the substitution $\overline{w} \mapsto Re^{-i\varphi}$ in the third equality. The last equality now follows as $\mathcal{L}_{wa}\left(R^{-1}e^{-i\varphi}\right)$ behaves at worst like $\log\left(R^{-1}e^{-i\varphi}\right)^k$ for small R and $k \in \mathbb{N}_0$. Then, as for $R \to 0$, $R\log\left(Re^{i\varphi}\right)^k \to 0$ for any k, it follows that the expression vanishes.

Collecting all terms we find that the integral (I) gives in total $-\mathcal{L}_{wa}(y)w_0(\overline{y})$. In the following, we are not going to write out the precise calculations after applying Stokes' theorem anymore as they are rather repetitive. In an abuse of notation we are suggestively going to write γ in the integral boundaries for an appropriate curve cutting out the problematic points of each term and going once around everything. With this we find for the integral of (II):

$$\frac{1}{2\pi i} \int_{z\in\mathbb{C}} \mathcal{L}_w(z) w_0(\overline{z}) \wedge w_a(z) \wedge w_z(y) = \frac{1}{2\pi i} \int_{\gamma} \mathcal{L}_{0w}(z) w_a(z) \wedge w_z(y) = \mathcal{L}_{0w}(y) w_a(y).$$

where in the first equality we used Remark 2.12 as well as the defining differential equation for single-valued polylogarithms. Combining all the above we have:

$$\frac{1}{2\pi i} \int_{z\in\mathbb{C}} \mathcal{L}_w(z) w_a(z) \wedge d\arg(|z|^2) \wedge d\arg(|z-y|^2) = -\mathcal{L}_{wa}(y) w_0(\overline{y}) + \mathcal{L}_{0w}(y) w_a(y).$$

Similarly to this, one finds that

$$\frac{1}{2\pi i} \int_{z_k\in\mathbb{C}} \mathcal{L}_w(z) w_a(\overline{z}) \wedge d\arg(|z|^2) \wedge d\arg(|z-y|^2) = -\mathcal{L}_{w0}(y) w_a(\overline{y}) + \mathcal{L}_{aw}(y) w_0(y).$$

By using the definition of $f(k+1)$ and integrating using the above we find

$$\begin{aligned}
f(k+1)(y) &= \frac{1}{2\pi i} \int_{z\in\mathbb{C}} f(k)(z) \wedge d\arg(|z|^2) \wedge d\arg(|z-y|^2) \\
= \mathcal{L}_{0^{k+1}}(y) w_1(y) &- \mathcal{L}_{0^k 1}(y) w_0(\overline{y}) + (-1)^{k+2} \mathcal{L}_{0^{k+1}}(y) w_1(\overline{y}) + (-1)^{k+1} \mathcal{L}_{10^k}(y) w_0(y) \\
&+ \sum_{n+m=k-1} \mathcal{L}_{0^n 10^{m+1}}(y) w_0(\overline{y}) (-1)^{m+2} \left(\binom{n+m+1}{n} + \binom{n+m+1}{m} \right) \\
&+ \mathcal{L}_{0^{n+1} 10^m}(y) w_0(y) (-1)^{m+1} \left(\binom{n+m+1}{n} + \binom{n+m+1}{m} \right).
\end{aligned}$$

Let us only consider the first part of the sum and the term $\mathcal{L}_{0^k 1}(y)$ then by substituting $m \mapsto$

$m-1$ we have

$$-\mathcal{L}_{0^k1}(y)w_0(\overline{y}) + \sum_{n+m=k-1} \mathcal{L}_{0^n10^{m+1}}(y)w_0(\overline{y})(-1)^{m+2}\left(\binom{n+m+1}{n} + \binom{n+m+1}{m}\right)$$
$$= -\mathcal{L}_{0^k1}w_0(\overline{y}) + \sum_{\substack{n+m-1=k-1\\ m>0}} \mathcal{L}_{0^n10^m}(y)w_0(\overline{y})(-1)^{m+1}\binom{n+m+1}{m}$$
$$= \sum_{n+m=k} \mathcal{L}_{0^n10^m}(y)w_0(\overline{y})(-1)^{m+1}\binom{n+m+1}{m}$$

where we used the substitution as well as $\binom{n+m}{n}+\binom{n+m}{m-1} = \binom{n+m+1}{m}$ in the first equality. Similarly, by substituting $n \mapsto n-1$ one shows for the second part of the sum and the term with $\mathcal{L}_{10^k}(y)$ that

$$(-1)^{k+1}\mathcal{L}_{10^k}(y)w_0(y) + \sum_{n+m=k-1} \mathcal{L}_{0^{n+1}10^m}(y)w_0(y)(-1)^{m+1}\left(\binom{n+m+1}{n} + \binom{n+m+1}{m}\right)$$
$$= \sum_{n+m=k} \mathcal{L}_{0^n10^m}(y)w_0(y)(-1)^{m+1}\binom{n+m+1}{n}$$

Combining these two results and plugging them in shows the formula for the case of $f(k+1)$ and thus concludes the induction. □

Prof of the second claim. The base case for $k=1$ is trivial as in this case the only possibility is that the edge $(z_2, 1)$ is the special edge and thus we have

$$\widetilde{f}(1)(z_2) = -\mathcal{L}_1(z_2).$$

For the induction step assume the formula holds for k. Let us write $z := z_{k+1}$ and $y := z_{k+2}$. We will first compute the integrals for the separate terms. Let $w \in \{0,1\}^*$ containing precisely one 1. We find for the integral

$$\frac{1}{2\pi i}\int_{z\in\mathbb{C}} \mathcal{L}_w(z)d\arg(|z|^2) \wedge d\arg(|z-y|^2) = \frac{1}{2\pi i}\int_{z\in\mathbb{C}} \mathcal{L}_w(z)(w_0(z) - w_0(\overline{z})) \wedge (w_y(z) - w_{\overline{y}}(\overline{z}))$$
$$= \frac{1}{2\pi i}\int_\gamma -\mathcal{L}_{w0}(z)w_{\overline{y}}(\overline{z}) - \mathcal{L}_{0w}(z)w_y(z) = \mathcal{L}_{0w}(y) - \mathcal{L}_{w0}(y).$$

In the induction step this integral can be used for the part where $\widetilde{f}$ is integrated over the next vertex and the special edge has already appeared before. Consider now the case where the special edge appears at this vertex going to 0. The integrals in question are then

$$\frac{1}{2\pi i}\int_{z\in\mathbb{C}} \mathcal{L}_w(z)w_0(z)\log\left(|z|^2\right)d\arg(|z-y|^2) = \frac{1}{2\pi i}\int_{z\in\mathbb{C}} -\mathcal{L}_w(z)\mathcal{L}_0(z)w_0(z) \wedge w_{\overline{y}}(\overline{z})$$
$$= \frac{1}{2\pi i}\int_{z\in\mathbb{C}} -\mathcal{L}_{w\sqcup\!\sqcup 0}(z)w_0(z) \wedge w_{\overline{y}}(\overline{z})$$
$$= \frac{1}{2\pi i}\int_{z\in\mathbb{C}} \left(-(n+1)\mathcal{L}_{0^{n+1}10^m}(z) - (m+1)\mathcal{L}_{0^n10^{m+1}}(z)\right)w_0(z) \wedge w_{\overline{y}}(\overline{z})$$
$$= -(n+1)\mathcal{L}_{0^{n+1}10^{m+1}}(y) - (m+1)\mathcal{L}_{0^n10^{m+2}}(y).$$

Similarly, one obtains

$$\frac{1}{2\pi i}\int_{z\in\mathbb{C}}\mathcal{L}_w(z)w_0(\overline{z})\log\Big(|z|^2\Big)d\arg(|z-y|^2)=-(n+1)\mathcal{L}_{0^{n+2}10^m}(y)-(m+1)\mathcal{L}_{0^{n+1}10^{m+1}}(y)$$
$$\frac{1}{2\pi i}\int_{z\in\mathbb{C}}\mathcal{L}_{0^k}(z)w_1(z)\log\Big(|z|^2\Big)d\arg(|z-y|^2)=-(k+1)\mathcal{L}_{0^{k+1}1}(y)$$
$$\frac{1}{2\pi i}\int_{z\in\mathbb{C}}\mathcal{L}_{0^k}(z)w_1(\overline{z})\log\Big(|z|^2\Big)d\arg(|z-y|^2)=-(k+1)\mathcal{L}_{10^{k+1}}(y).$$

Finally, the last integral we need to compute is the case of the special edge appearing at this vertex and going to the next vertex which has not been integrated yet. Let $w\in\{0,1\}^*$ with at most one 1 and $a\in\{0,1\}$. Then the integral we consider is

$$\begin{aligned}\frac{1}{2\pi i}\int_{z\in\mathbb{C}}\mathcal{L}_w(z)w_a(z)\log\Big(|z-y|^2\Big)d\arg(|z|^2)&=\frac{1}{2\pi i}\int_{z\in\mathbb{C}}-\mathcal{L}_w(z)\mathcal{L}_0(z-y)w_a(z)\wedge w_0(\overline{z})\\&=\underbrace{\frac{1}{2\pi i}\int_\gamma-\mathcal{L}_{wa}(z)\mathcal{L}_0(z-y)w_0(\overline{z})}_{=0}+\frac{1}{2\pi i}\int_{z\in\mathbb{C}}\mathcal{L}_{wa}(z)w_y(z)\wedge w_0(\overline{z})\\&=\frac{1}{2\pi i}\int_\gamma\mathcal{L}_{0wa}(z)w_y(z)=\mathcal{L}_{0wa}(y).\end{aligned}$$

where we used partial integration in the second equality and the marked term vanishes as $\mathcal{L}_{wa}(0)=0$. Similarly, one finds

$$\frac{1}{2\pi i}\int_{z\in\mathbb{C}}\mathcal{L}_w(z)w_a(\overline{z})\log\Big(|z-y|^2\Big)d\arg(|z|^2)=\mathcal{L}_{aw0}(y).$$

With these integrals now pre-computed we find for $\widetilde{f}$:

$$\begin{aligned}\widetilde{f}(k+1)(y)=&\int_{z\in\mathbb{C}}\widetilde{f}(k)(z)\wedge d\arg(|z|^2)\wedge d\arg(|z-y|^2)\\&+\log\Big(|z|^2\Big)f(k-1)(z)\wedge d\arg(|z-y|^2)-\log\Big(|z-y|^2\Big)f(k-1)(z)\wedge d\arg(|z|^2)\\=&(2k-1)\sum_{n+m=k-1}(\mathcal{L}_{0^{n+1}10^m}(y)-\mathcal{L}_{0^n10^{m+1}}(y))(-1)^{m+1}\binom{k-1}{n}-k\mathcal{L}_{0^k1}(y)-(-1)^kk\mathcal{L}_{10^k}(y)\\&+\sum_{n+m=k-2}(-1)^{m+2}\Bigg((n+1)\binom{k-1}{m}\mathcal{L}_{0^{n+2}10^m}(y)\\&+\left((n+1)\binom{k-1}{n}+(m+1)\binom{k-1}{m}\right)\mathcal{L}_{0^{n+1}10^{m+1}}(y)+(m+1)\binom{k-1}{n}\mathcal{L}_{0^n10^{m+2}}(y)\Bigg)\\&-\mathcal{L}_{0^k1}(y)-(-1)^k\mathcal{L}_{10^k}(y)+\sum_{n+m=k-2}\mathcal{L}_{0^{n+1}10^{m+1}}(y)(-1)^{m+2}\left(\binom{k-1}{n}+\binom{k-1}{m}\right).\end{aligned}$$

Substituting n and m such that everywhere the word $\mathcal{L}_{0^{n+i}10^{m+j}}(y)$ becomes $\mathcal{L}_{0^n10^m}(y)$ and then separating out the terms for $m=0$ and $n=0$ where they appear we obtain

$$(2k-1)\sum_{\substack{n+m=k\\n\geq 1,m\geq 1}}(-1)^{m+1}\mathcal{L}_{0^n10^m}(y)\binom{k}{n}-(2k+1)(\mathcal{L}_{0^k1}(y)-(-1)^{k+1}\mathcal{L}_{10^k}(y))$$
$$+\sum_{\substack{n+m=k\\n\geq 1,m\geq 1}}\mathcal{L}_{0^n10^m}(y)(-1)^{m+1}\left((n+1)\binom{k-1}{n-1}+(m+1)\binom{k-1}{m-1}\right)$$
$$+\sum_{\substack{n+m=k\\n\geq 2,m\geq 1}}\mathcal{L}_{0^n10^m}(y)(-1)^{m+2}(n-1)\binom{k-1}{n-1}+\sum_{\substack{n+m=k\\n\geq 1,m\geq 2}}\mathcal{L}_{0^n10^m}(y)(-1)^{m+2}(m-1)\binom{k-1}{m-1}.$$

Notice that both sums in the last line can be extended to $n=1$ and $m=1$ respectively as these terms are 0. Thus, gathering together the second and third line we obtain

$$(2k-1)\sum_{\substack{n+m=k\\n\geq 1,m\geq 1}}(-1)^{m+1}\mathcal{L}_{0^n10^m}(y)\binom{k}{n}-(2k+1)(\mathcal{L}_{0^k1}(y)-(-1)^{k+1}\mathcal{L}_{10^k}(y))$$
$$+\sum_{\substack{n+m=k\\n\geq 1,m\geq 1}}\mathcal{L}_{0^n10^m}(y)(-1)^{m+1}\left(2\binom{k-1}{n-1}+2\binom{k-1}{m-1}\right)$$
$$=(2k+1)\sum_{\substack{n+m=k\\n\geq 1,m\geq 1}}(-1)^{m+1}\mathcal{L}_{0^n10^m}(y)\binom{k}{n}-(2k+1)(\mathcal{L}_{0^k1}(y)-(-1)^{k+1}\mathcal{L}_{10^k}(y))$$
$$=(2k+1)\sum_{n+m=k}(-1)^{m+1}\mathcal{L}_{0^n10^m}(y)\binom{k}{n}.$$

where we used $\binom{k-1}{n-1}+\binom{k-1}{m-1}=\binom{k}{n}$ in the first equality. This concludes the proof. □

2.5 Drinfel'd associators and the Grothendieck-Teichmüller Lie algebra

In the 1980s Drinfel'd develeoped most of the following notions in [11]. Here we mostly follow M. Felder's exposition in [12].

Definition 2.20. A *Drinfel'd associator* is a pair $(\mu,\Phi)\in\mathbb{K}^\times\times\mathbb{K}\langle\langle x,y\rangle\rangle$ such that Φ is group-like, that is $\Delta(\Phi)=\Phi\widehat{\otimes}\Phi$ and satisfies the following equations

$$\Phi(x,y)=\phi(x,y)^{-1}$$
$$e^{\frac{\mu}{2}A}\Phi(x,y)e^{\frac{\mu}{2}B}\Phi(y,z)e^{\frac{\mu}{2}C}\Phi(z,x)=1$$
$$\Phi(t_{23},t_{34})\Phi(t_{12}+t_{13},t_{24}+t_{34})\Phi(t_{12},t_{23})=\Phi(t_{12},t_{23}+t_{24})\Phi(t_{13}+t_{23},t_{34}).$$

where $A+B+C=0$ and the last equation takes values in the universal enveloping algebra of the Drinfel'd-Kohno Lie algebra $\mathfrak{t}_4$. We denote the set of these associators by DAss and write $\Phi(w)$ for the coefficient of w in the series expansion of Φ.

Here the Drinfel'd-Kohno Lie algebra is defined as follows:

Definition 2.21. Let $k\geq 2$. Then the *Drinfel'd-Kohno Lie algebra* $\mathfrak{t}_k$ is the free Lie algebra spanned by generators t_{ij} with $1\leq i\neq j\leq k$, modulo the following relations:

$$t_{ij}=t_{ji}\qquad [t_{ij},t_{kl}]=0\text{ for }\{i,j\}\cap\{k,l\}=\varnothing\qquad [t_{ij},t_{ik}+t_{jk}]=0\text{ for }k\neq i,j.$$

Remark 2.22. Initially the Drinfel'd associators were required to satisfy a fourth set of equations known as hexagon equations

$$\begin{aligned}e^{\frac{\mu(t_{13}+t_{23})}{2}} &= \Phi\left(t_{13}, t_{12}\right) e^{\frac{\mu t_{13}}{2}} \Phi\left(t_{13}, t_{23}\right)^{-1} e^{\frac{\mu t_{23}}{2}} \Phi\left(t_{12}, t_{23}\right) \\ e^{\frac{\mu(t_{12}+t_{13})}{2}} &= \Phi\left(t_{23}, t_{13}\right)^{-1} e^{\frac{\mu t_{13}}{2}} \Phi\left(t_{12}, t_{13}\right) e^{\frac{\mu t_{12}}{2}} \Phi\left(t_{12}, t_{23}\right)^{-1}.\end{aligned}$$

However, Furushu showed in [13] that the heptagon equation (that is the last equation in Definition 2.20) already implies the hexagon equations.

Importantly, in the above definition the μ is required to be unequal 0. The special elements for the case of $\mu = 0$ give the following group:

Definition 2.23. The *Grothendieck-Teichmüller group* GRT_1 is the pro-unipotent group whose elements are solutions Φ of the equations from Definition 2.20 for $\mu = 0$. For $\Phi, \Phi' \in \mathsf{GRT}_1$ the group operation is given by

$$(\Phi \cdot \Phi')(x, y) = \Phi(x, y)\Phi'(x, \Phi(x, y)^{-1} y\Phi(x, y)),$$

where the product on the right is the usual product in $\mathbb{K}\langle\langle x, y\rangle\rangle$.

This group acts freely and transitively on the set of Drinfel'd associators DAss via the action

$$\begin{aligned}\mathsf{GRT}_1 \times \mathrm{DAss} &\to \mathrm{DAss} \\ (\Psi, (\mu, \Phi)) &\mapsto (\mu, \Psi \cdot \Phi)\end{aligned}$$

where $\cdot$ is given in the same way as the group operation on GRT_1.

Finally, there exists a pro-nilpotent Lie algebra $\mathfrak{grt}_1$ such that GRT_1 is the exponential of $\mathfrak{grt}_1$, that is $\mathsf{GRT}_1 = \exp(\mathfrak{grt}_1)$:

Definition 2.24. Let the *Grothendieck-Teichmüller Lie algebra* $(\mathfrak{grt}_1, \{\cdot, \cdot\})$ be the Lie algebra of series $\psi \in \widehat{\mathbb{F}}(x, y)$ such that

$$\begin{aligned}\psi(x, y) &= -\psi(y, x) \\ \psi(x, y) + \psi(y, z) + \psi(z, x) &= 0 \\ \psi(t_{12}, t_{23}) + \psi(t_{12} + t_{13}, t_{24} + t_{34}) + \psi(t_{23}, t_{34}) &= \psi(t_{12}, t_{23} + t_{24}) + \psi(t_{13} + t_{23}, t_{34}).\end{aligned}$$

where $x + y + z = 0$ and as before the last equation takes values in $\mathfrak{t}_4$. The Lie bracket on $\mathfrak{grt}_1$ is given by the *Ihara bracket*:

$$[\psi, \psi']_{\mathrm{Ih}}(x, y) = [\psi(x, y), \psi'(x, y)] + D_\psi \psi'(x, y) - D_{\psi'}\psi(x, y).$$

Here D_ψ is the derivation given by sending x to x and y to $[y, \psi]$ where $[\cdot, \cdot]$ is the standard bracket in $\widehat{\mathbb{F}}(x, y)$.

Definition 2.25. Moreover, $\mathfrak{grt}_1$ also acts on DAss by

$$\begin{aligned}\mathfrak{grt}_1 \times \mathrm{DAss} &\to \mathrm{DAss} \\ (\gamma(x, y), (\mu, \Phi)) &\mapsto (\mu, \gamma(x, y)\Phi(x, y) + [y, \gamma]\partial_y \Phi(x, y)).\end{aligned}$$

Here the product is the usual product in $\mathbb{K}\langle\langle x, y\rangle\rangle$ and $[y, \gamma]\partial_y$ is the derivation sending x to 0 and y to $[y, \gamma]$.

As we are going to need this action rather often we best illustrate the action of the derivation by an example:

Example 2.26. Let $w \in \{0,1\}^*$. Consider the derivation $[y,w]\partial_y$ acting on xyx^2yx. Then

$$[y,w]\partial_y(xyx^2yx) = x[y,w]x^2yx + xyx^2[y,w]x = xywx^2yx - xwyx^2yx + xyx^2ywx - xyx^2wyx.$$

Now we can again introduce the KZ-associator which was first defined by Drinfel'd in [11].

Definition 2.27. The KZ-associator is given by

$$\Phi_{KZ}(x,y) := \sum_{w \in \{x,y\}^*} \frac{\zeta(w)}{(2\pi i)^{|w|}} w.$$

Its counterpart the anti-KZ-associator is then given by

$$\Phi_{\overline{KZ}}(x,y) := \Phi_{KZ}(-x,-y) = \sum_{x \in \{x,y\}^*} (-1)^{|w|} \frac{\zeta(w)}{(2\pi i)^{|w|}} w.$$

Both Φ_{KZ} and $\Phi_{\overline{KZ}}$ are associators in the sense of Definition 2.20.

Remark 2.28. Remember that from Theorem 2.13 it follows that Φ^{sv}_{KZ} is an element of $\mathfrak{grt}_1$. This can easily be seen from the above definition as in a Drinfel'd associator μ only appears as the coefficient of the term $[x,y]$. In the case of the KZ-associator the coefficient for this is given by $-\frac{\zeta(2)}{4\pi^2}$. However, as $\zeta_{\text{sv}}(2) = 0$ it follows that the coefficient of $[x,y]$ in Φ^{sv}_{KZ} is 0 and thus that $\mu = 0$ for Φ^{sv}_{KZ}. Therefore, Φ^{sv}_{KZ} is an element of $\mathfrak{grt}_1$ as it fulfills the required equations by virtue of Φ_{KZ} being a Drinfel'd associator and as the single-valued MZVs (conjecturally) satisfy the same relations as multiple zeta values.

3 Calculating τ^t to depth 3

Let us write

$$\text{ad}_x^k(y) = [\underbrace{x,[x,\ldots,[x}_{k-\text{times}},y]]].$$

The idea of this section is to use the defining equation

$$\Phi_{\overline{KZ}} = \psi \cdot \Phi_{KZ} \tag{2}$$

to calculate the τ_{2j+1}. For this we are going to show that the τ_{2j+1} up to depth 3 can be written as follows

$$\tau_{2j+1} = c_{2j}\,\text{ad}_x^{2j}(y) + \sum_{\substack{0 \le \alpha < \beta \\ \alpha+\beta = 2j-1}} c_{\alpha,\beta} \left[\text{ad}_x^\alpha(y), \text{ad}_x^\beta(y)\right] + \sum_{\substack{\beta < \gamma, \alpha \le \gamma \\ \alpha+\beta+\gamma = 2j-2}} c_{\alpha,\beta,\gamma} \left[\text{ad}_x^\alpha(y), \left[\text{ad}_x^\beta(y), \text{ad}_x^\gamma(y)\right]\right].$$

Then for every word w of depth 1, 2 or 3 we get an equation from (2) by only considering the terms that contribute w. It turns out that by choosing the right words w this gives a system of linear equations from which the $c_{2n}, c_{\alpha,\beta}, c_{\alpha,\beta,\gamma}$ can be recovered.

The case for depth 1 has been done by M. Felder in [12] (Lemma 5.6) and gives the following:

$$c_{2n} = \frac{2}{I_1^n} \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}.$$

where we define

$$I_t^n := \int_0^t (x(x-1))^{2n}\,\mathrm{d}x$$

which for $t=1$ equals $\frac{((2n)!)^2}{(4n+1)!}$. Moreover, we are going to need the following two definitions

$$J_t^{l,m} = \int_0^t \int_0^x (x(x-1))^{2l}(y(y-1))^{2m}\,\mathrm{d}y\,\mathrm{d}x$$

and

$$K_t^{l,m,h} = \int_0^t \int_0^x \int_0^y (x(x-1))^{2l}(y(y-1))^{2m}(z(z-1))^{2h}\,\mathrm{d}z\,\mathrm{d}y\,\mathrm{d}x\,.$$

3.1 The depth 2 coefficients $c_{\alpha,\beta}$

In [12] it was shown that when considering the depth 2 part of the defining equation (2) for a word $w = x^a y x^b y x^c$ that is

$$\left(1 + I_1^n \sum_{\alpha,\beta} c_{\alpha,\beta}\left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right] + \sum_{s\in\mathbb{N}} I_1^s c_{2s}\,\mathrm{ad}_x^{2s}(y) + \dots\right)$$
$$\cdot\left(1 + u_{x^ayx^byx^c} x^a y x^b y x^c + \sum_{p,q\in\mathbb{N}_0} u_{x^pyx^q} x^p y x^q + \dots\right) = -u_{x^ayx^byx^c} x^a y x^b y x^c$$

the terms contributing the word w give the following equation:

Lemma 3.1. *Fix $n \geq 1$ and let $a,b,c \in \mathbb{N}_0$ such that $a+b+c+2 = 2n+1$. The coefficients $c_{\alpha,\beta}$ satisfy the following set of equations.*

$$\begin{aligned}
-2u_{x^ayx^byx^c} = I_1^n &\sum_{\substack{0\le\alpha<\beta\\ \alpha+\beta+2=2n+1}} c_{\alpha,\beta}\left(\binom{\alpha}{a}\binom{\beta}{c}(-1)^{a+\beta-c} - \binom{\alpha}{c}\binom{\beta}{a}(-1)^{a+\alpha-c}\right)\\
&+ \sum_{\substack{p\in\mathbb{N}_0,s\in\mathbb{N}\\ 2s=b+a-p}} I_1^s c_{2s}\left(\binom{2s}{a}(-1)^a - \binom{2s}{b}(-1)^b\right) u_{x^pyx^c}\\
&+ \sum_{\substack{q\in\mathbb{N}_0,s\in\mathbb{N}\\ 2s=b+c-q}} I_1^s c_{2s}\binom{2s}{b}(-1)^b u_{x^ayx^q}.
\end{aligned}$$

This proof mostly relies on the application of the following identities, which we will heavily use later on:

Remark 3.2. To pass from $\widehat{\mathbb{F}}_{\mathrm{Lie}}(x,y)$ to $\mathbb{K}\langle\langle x,y\rangle\rangle$ one sets $[x,y] = xy - yx$. The following identities hold:

$$\mathrm{ad}_x^\alpha(y) = (-1)^\alpha \sum_{i=0}^{\alpha}\binom{\alpha}{i}(-1)^i x^i y x^{\alpha-i}$$

$$[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)] = (-1)^{\alpha+\beta}\sum_{i=0}^{\alpha}\sum_{j=0}^{\beta}\binom{\alpha}{i}\binom{\beta}{j}(-1)^{i+j}\left(x^i y x^{\alpha-i+j} y x^{\beta-j} - x^j y x^{\beta-j+i} y x^{\alpha-j}\right)$$

$$\begin{aligned}
\left[\mathrm{ad}_x^\alpha(y), \left[\mathrm{ad}_x^\beta(y), \mathrm{ad}_x^\gamma\right]\right] = (-1)^{\alpha+\beta+\gamma}&\sum_{i=0}^{\alpha}\sum_{j=0}^{\beta}\sum_{k=0}^{\gamma}\binom{\alpha}{i}\binom{\beta}{j}\binom{\gamma}{k}(-1)^{i+j+k}\Big(x^i y x^{\alpha-i+j} y x^{\beta-j+k} y x^{\gamma-k}\\
&-x^j y x^{\beta-j+k} y x^{\gamma-k+i} y x^{\alpha-i} - x^i y x^{\alpha-i+k} y x^{\gamma-k+j} y x^{\beta-j} + x^k y x^{\gamma-k+j} y x^{\beta-j+i} y x^{\alpha-i}\Big)
\end{aligned}$$

For the terms contributing the $c_{\alpha,\beta}$ in the above Lemma we find:

Lemma 3.3. *Let $n \in \mathbb{N}$. For $a \in \{0, \dots, n-1\}$ and $c = 2n-1-a$ the following holds*

$$\sum_{\substack{0 \le \alpha < \beta \\ \alpha+\beta+2=2n+1}} c_{\alpha,\beta} \left(\binom{\alpha}{a}\binom{\beta}{c}(-1)^{a+\beta-c} - \binom{\alpha}{c}\binom{\beta}{a}(-1)^{a+\alpha-c} \right) = (-1)^a c_{a,c}. \tag{3}$$

Proof. By definition $a + c = 2n - 1$. We can rewrite the first term of binomial coefficients as

$$\binom{\alpha}{a}\binom{\beta}{c} = \binom{\alpha}{a}\binom{2n-1-\alpha}{2n-1-a}$$

by using the definition of β and c. However, here if $\alpha < a$ the first factor is 0 and if $\alpha > a$ the second factor vanishes. In the case of $\alpha = a$ clearly the expression equals 1. Thus, we have that

$$\binom{\alpha}{a}\binom{\beta}{c} = \delta_{\alpha a}\delta_{\beta c}.$$

Similarly, for the second term we have

$$\binom{\alpha}{c}\binom{\beta}{a} = \binom{\alpha}{c}\binom{2n-1-\alpha}{2n-1-c}$$

by using the definition of β and a. Through the same observation as above one finds

$$\binom{\alpha}{c}\binom{\beta}{a} = \delta_{\alpha c}\delta_{\beta a}.$$

Coming back to the initial equation (3) it reduces to

$$\sum_{\substack{0 \le \alpha < \beta \\ a+\beta+2=2n+1}} c_{\alpha,\beta} \left(\delta_{\alpha a}\delta_{\beta c}(-1)^{\alpha+\beta-c} - \delta_{\alpha c}\delta_{\beta a}(-1)^{a+\alpha-c} \right).$$

Now notice that from our definition of a and c it follows that $a < c$ paired with $\alpha < \beta$ this results in the vanishing of the second summand. Therefore, we are left with

$$\sum_{\substack{0 \le \alpha < \beta \\ a+\beta+2=2n+1}} c_{\alpha,\beta}\delta_{\alpha a}\delta_{\beta c}(-1)^{\alpha+\beta-c} = c_{a,c}(-1)^{a+c-c} = (-1)^a c_{a,c}$$

which concludes the proof. □

From the above result we immediately get the following formula for the $c_{\alpha,\beta}$:

Corollary 3.4. *Let $n \in \mathbb{N}$. For $a \in \{0, \dots, n-1\}$ and $c = 2n-1-a$ we have*

$$c_{a,c} = \frac{(-1)^{a+1}}{I_1^n} \left(2u_{x^a y^2 x^c} + \sum_{\substack{p \in \mathbb{N}_0, s \in \mathbb{N} \\ 2s=a-p}} I_1^s c_{2s} \left(\binom{2s}{a}(-1)^a - 1 \right) u_{x^p y x^c} + \sum_{\substack{q \in \mathbb{N}_0, s \in \mathbb{N} \\ 2s=c-q}} I_1^s c_{2s} u_{x^a y x^q} \right) \tag{4}$$

Our next goal is to simplify this expression. By plugging in the definitions of c_{2n}, I_1^{2n} and $u_{x^i y x^j}$ as well as using the parity theorem for multiple zeta values we get the following final form:

Theorem 3.5. *Let $n \in \mathbb{N}$ and let $\alpha \in \{0, \dots, n-1\}$ and $\beta = 2n-1-\alpha$. Then the following holds:*

$$c_{\alpha,\beta} = \frac{-(4n+1)!}{((2n)!)^2} \left(\binom{2n}{\alpha} - \binom{2n}{\alpha+1} + (-1)^{\alpha+1} \right) \frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}.$$

The proof of this theorem mostly relies on the parity theorem 2.7 and the binomial identities given in Lemma 1.3.

Proof. Let us first simplify the second term in the sum of equation (4):

$$\sum_{\substack{p\in\mathbb{N}_0,s\in\mathbb{N}\\2s=a-p}} I_1^s c_{2s}\left(\binom{2s}{a}(-1)^a-1\right)u_{x^pyx^c}$$
$$=2\sum_{\substack{s\in\mathbb{N},\\p=a-2s\geq 0}}\frac{\zeta(2s+1)}{(2\pi i)^{2s+1}}\left(\binom{2s}{a}(-1)^a-1\right)(-1)^{c+1}\binom{p+c}{p}\frac{\zeta(p+c+1)}{(2\pi i)^{p+c+1}}$$
$$=2\sum_{\substack{s\in\mathbb{N}\\a\geq 2s}}\left(\delta_{2s,a}-(-1)^a\binom{a+c-2s}{c}\right)\frac{\zeta(2(n-s))\zeta(2s+1)}{(2\pi i)^{2n+1}} \tag{†}$$

where for the second equality we used that $\binom{2s}{a}=0$ for $a>2s$ and 1 for $a=2s$ in which case $(-1)^a=1$ as well as that $\binom{a+c-2s}{c}=1$ for $a=2s$. Moreover,

$$\binom{p+c}{p}=\binom{a+c-2s}{a-2s}=\binom{a+c-2s}{c}$$

by using that $\binom{n}{k}=\binom{n}{n-k}$. Finally, as $a+c=2n-1$ we have that $(-1)^{c+1}=(-1)^{2n-1-a+1}=(-1)^a$ as well as $\zeta(p+c+1)=\zeta(a+c-2s+1)=\zeta(2(n-s))$.

For the third term in the sum of equation (4) we similarly get:

$$\sum_{\substack{q\in\mathbb{N}_0,s\in\mathbb{N}\\2s=c-q}} I_1^s c_{2s}u_{x^ayx^q}=2\sum_{\substack{s\in\mathbb{N}\\q=c-2s\geq 0}}\frac{\zeta(2s+1)}{(2\pi i)^{2s+1}}(-1)^{q+1}\binom{a+q}{a}\frac{\zeta(a+q+1)}{(2\pi i)^{a+q+1}}$$
$$=2(-1)^a\sum_{\substack{s\in\mathbb{N}\\c\geq 2s}}\binom{a+c-2s}{a}\frac{\zeta(2s+1)\zeta(2(n-s))}{(2\pi i)^{2n+1}}. \tag{††}$$

Finally, we can investigate the term $2u_{x^ay^2x^c}$ by using the parity Theorem 2.7 as well as Lemma 2.3 we find:

$$2u_{x^ay^2x^c}=2(-1)^c\frac{\zeta(x^ay^2x^c)}{(2\pi i)^{a+c+2}}=2(-1)^c\sum_{k=0}^{c}\binom{a+c-k}{a}\frac{\zeta(a+c-k+1,k+1)}{(2\pi i)^{2n+1}}$$
$$=2(-1)^c\sum_{k=0}^{c}\binom{a+c-k}{a}(-1)^{k+1}\sum_{s=0}^{n-1}\left[\binom{2n-2s}{k}+\binom{2n-2s}{a+c-k}-\delta_{a+c-k+1,2s}+(-1)^{k+1}\delta_{s,0}\right]$$
$$\frac{\zeta(2s)\zeta(2n+1-2s)}{(2\pi i)^{2n+1}}=2(-1)^c\sum_{s=1}^{n}\frac{\zeta(2(n-s))\zeta(2s+1)}{(2\pi i)^{2n+1}}\sum_{k=0}^{c}(-1)^{k+1}\binom{a+c-k}{a}$$
$$\left[\underbrace{\binom{2s}{a+c-k}}_{(I)}+\underbrace{\binom{2s}{k}}_{(II)}-\underbrace{\delta_{2s,k}}_{(III)}-(-1)^{k+1}\delta_{n,u}\right] \tag{♡}$$

where in the last equality we substituted s with $n-s$. Notice now that if $s\neq n-1$ then $\zeta(2(n-s))$ is an even zeta value unequal $\zeta(0)$. Thus, as all terms in (†) and (††) contain even zeta values and we want to show that the terms for $s\neq n-1$ cancel those. We find for the terms (III) that

$$
\begin{aligned}
&2(-1)^c \sum_{s=1}^{n-1} \sum_{k=0}^{c} (-1)^{k+1} \binom{a+c-k}{a} (-\delta_{2s,k}) \frac{\zeta(2(n-s))\zeta(2s+1)}{(2\pi i)^{2n+1}} \\
&= 2(-1)^c \sum_{s=1}^{n-1} \binom{a+c-2s}{a} \frac{\zeta(2(n-s))\zeta(2s+1)}{(2\pi i)^{2n+1}}.
\end{aligned}
$$

Now as for $2s > c$ the binomial coefficient $\binom{a+c-2s}{a}$ is 0, the sum of s from 1 to $n-1$ is equal to the sum $s \in \mathbb{N}, c \geq 2s$. Moreover, as $(-1)^c = (-1)^{2n-1-a} = -(-1)^a$ the sign of this expression is opposite to (††) and thus the two expressions cancel.

Let us next consider the terms (II). Here we have

$$
\sum_{k=0}^{c} (-1)^{k+1} \binom{a+c-k}{a} \binom{2s}{k} = \binom{c+a}{k=0} (-1)^{k+1} \binom{a+c-k}{a} \binom{2s}{k} = -\binom{c+a-2s}{c}
$$

where in the first equality we used that for $k > c$ the binomial coefficient $\binom{a+c-k}{a}$ is 0 and in the second equality we used the second identity from Lemma 1.3 with $\overline{r} = c$, $\overline{s} = 2s$, $\overline{m} = a$, $\overline{k} = k$ and $\overline{t} = 0$. From this we get:

$$
\begin{aligned}
&2(-1)^c \sum_{s=1}^{n-1} \sum_{k=0}^{c} (-1)^{k+1} \binom{a+c-k}{a} \binom{2s}{k} \frac{\zeta(2(n-s))\zeta(2s+1)}{(2\pi i)^{2n+1}} \\
&= 2(-1)^{c+1} \sum_{s=1}^{n-1} \binom{a+c-2s}{c} \frac{\zeta(2(n-s))\zeta(2s+1)}{(2\pi i)^{2n+1}}.
\end{aligned}
$$

Once again for $2s > a$ the binomial coefficient $\binom{a+c-2s}{a}$ is 0 and the sum of s from 1 to $n-1$ is equal to the sum $s \in \mathbb{N}, a \geq 2s$. Moreover, as $(-1)^{c+1} = (-1)^{2n-1-a+1} = (-1)^a$ the sign of this expression is opposite to the sign of the terms corresponding to the $(-1)^a$ in (†) and thus the two expressions cancel.

Finally, we consider the terms (I). Here,

$$
\begin{aligned}
\sum_{k=0}^{c} (-1)^{k+1} \binom{a+c-k}{a} \binom{2s}{a+c-k} &= (-1)^{c+1} \sum_{k=0}^{c} (-1)^k \binom{a+k}{a} \binom{2s}{a+k} \\
&= (-1)^{c+1} \sum_{k=0}^{c} (-1)^k \binom{2s}{a} \binom{2s-a}{k}
\end{aligned}
$$

where in the first equality we substituted $c-k$ with k and in the second equality we used the first identity from Lemma 1.3 with $\overline{h} = a$, $\overline{k} = k$ and $\overline{n} = 2s$. Notice that for $s \leq n-1$ we have that $2s - a \leq c$ as this is equal to $2s \leq a + c = 2n - 1$. We distinguish the following cases:

$$
(-1)^{c+1} \sum_{k=0}^{c} (-1)^k \binom{2s}{a} \binom{2s-a}{k} = \begin{cases} 0 & a > 2s \\ (-1)^{c+1} & a = 2s \\ 0 & a < 2s \end{cases}
$$

where the first case follows as for $a > 2s$, $\binom{2s}{a} = 0$. In the second case $a = 2s$, $\binom{2s-a}{k}$ is 0 for all k but $k = 0$ and in this case equals 1. In the last case $a < 2s$ we used that for $k > 2s - a$, $\binom{2s-a}{k} = 0$ to change the upper bound of the summation and then used the third identity from Lemma 1.3 with $\overline{n} = 2s - a$ and $\overline{j} = k$ to obtain that this vanishes. Using that $c + 1 = 2n - a$

we find that this reduces to $(-1)^a\delta_{2s,a}$. From this we obtain:

$$\begin{aligned}
&2(-1)^c\sum_{s=1}^{n-1}\sum_{k=0}^{c}(-1)^{k+1}\binom{a+c-k}{a}\binom{2s}{a+c-k}\frac{\zeta(2(n-s))\zeta(2s+1)}{(2\pi i)^{2n+1}}\\
&=2\sum_{s=1}^{n-1}(-1)^{c+a}\delta_{2s,a}\frac{\zeta(2(n-s))\zeta(2s+1)}{(2\pi i)^{2n+1}}
\end{aligned}$$

which as $a+c=2n-1$ is odd has exactly the opposite sign of the term in (†) corresponding to $\delta_{2s,a}$ and thus cancels.

Therefore, we have shown that in equation (4) the terms of (†) and (††) cancel with the terms of (♡) for $s \neq n$ and we have that

$$\begin{aligned}
c_{a,c}&=\frac{(-1)^a}{2I_1^{2n}}\left(2(-1)^c\sum_{k=0}^{c}(-1)^{k+1}\binom{2n-1-k}{a}\left(\binom{2n}{2n-1-k}+\binom{2n}{k}+(-1)^{k+1}\right)\right)\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}\\
&=\frac{-(4n+1)!}{((2n)!)^2}\left(\sum_{k=0}^{c}\binom{2n-(k+1)}{a}\left(\binom{2n+1}{k+1}(-1)^k-1\right)\right)\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}
\end{aligned}$$

where in the first equality we used that $a+c=2n-1$ and $\zeta(0)=-\frac{1}{2}$. For the second equality we plugged in the definition of I_1^{2n}, used that $a+c+1=2n$ and thus $(-1)^{a+c+1}=1$ as well as the following

$$\binom{2n}{2n-1-k}+\binom{2n}{k}=\binom{2n}{k+1}+\binom{2n}{k}=\binom{2n+1}{k+1}$$

where we use the identity $\binom{\overline{n}}{\overline{k}}=\binom{\overline{n}}{\overline{n}-\overline{k}}$ and $\binom{\overline{n}}{\overline{k}+1}+\binom{\overline{n}}{\overline{k}}=\binom{\overline{n}+1}{\overline{k}+1}$. Going further we can use the following two rearrangements to prove the result: We have that

$$\sum_{k=0}^{c}\binom{2n-(k+1)}{a}=\sum_{k=0}^{c}\binom{a+c-k}{c-k}=\sum_{k=0}^{c}\binom{a+k}{k}=\binom{a+c+1}{c}=\binom{2n}{c}$$

where in the second to last equality we used the fourth identity from Lemma 1.3. For the product of binomial coefficients we get:

$$\begin{aligned}
&\sum_{k=0}^{c}(-1)^k\binom{2n-(k+1)}{a}\binom{2n+1}{k+1}=-\sum_{k=1}^{2n}(-1)^k\binom{2n-k}{a}\binom{2n+1}{k}\\
&=-\binom{2n-(2n+1)}{2n-a}+\binom{2n}{a}=\binom{1+2n-a-1}{2n-a}(-1)^a+\binom{2n}{a}=\binom{2n}{a}-(-1)^a
\end{aligned}$$

where in the first equality we used that $2n-k=a+c+1-k<a$ for $k>c+1$ and therefore those terms vanish. In the second equality we used the second identity from Lemma 1.3 with $\overline{m}=a$, $\overline{r}=2n$, $\overline{s}=2n+1$ and $\overline{r}=0$. Finally, in the third equality we used the sixth identity from Lemma 1.3. Plugging those two rearrangements into the above equation and substituting $\alpha=a$ and $\beta=c$ yields the desired result. □

Example 3.6. Calculating the values of $c_{\alpha,\beta}$ for small n gives

$$c_{0,1}=60\frac{\zeta(3)}{(2\pi i)^3}$$

$$c_{1,2}=630\frac{\zeta(5)}{(2\pi i)^5}\qquad c_{0,3}=2520\frac{\zeta(5)}{(2\pi i)^5}$$

$$c_{2,3}=72072\frac{\zeta(7)}{(2\pi i)^7}\qquad c_{1,4}=96096\frac{\zeta(7)}{(2\pi i)^7}\qquad c_{0,5}=72072\frac{\zeta(7)}{(2\pi i)^7}$$

for $n = 1, 2, 3$ respectively. A full implementation of this can also be found in the code described in Appendix C.

Finally with this expression we can find the coefficient of an odd-length depth 2 word w in τ^t as:

Proposition 3.7. *Let $w = x^a y x^b y x^c$ be an odd-length depth 2 word. Then*

$$\tau\mid_w = \frac{(t(t-1))^{|w|-1}}{I_1^{|w|-1}}\left((-1)^{a+1}\binom{2n}{a} + (-1)^b\binom{2n}{b} + (-1)^{c+1}\binom{2n}{c}\right)\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}.$$

Proof. Let $w = x^a y x^b y x^c$ and let $2n+1$ be the length of w. Then w only appears in τ_{2n+1}. From the proof of Lemma 3.3 we know that the coefficient of w in τ_{2n+1} is given by

$$\sum_{\substack{0\le\alpha<\beta \\ \alpha+\beta+2=2n+1}} c_{\alpha,\beta}\left(\binom{\alpha}{a}\binom{\beta}{c}(-1)^{a+\beta-c} - \binom{\alpha}{c}\binom{\beta}{a}(-1)^{a+\alpha-c}\right).$$

Plugging in the expression for $c_{a,c}$ we get

$$\frac{1}{I_1^{2n}}\frac{\zeta(2n+1)}{(2\pi i)^{2n+1}}\sum_{\substack{0\le\alpha<\beta \\ \alpha+\beta+2=2n+1}}\left(\binom{2n}{\beta} - \binom{2n}{\alpha} + (-1)^\alpha\right)\left(\binom{\alpha}{a}\binom{\beta}{c}(-1)^{a+\beta-c} - \binom{\alpha}{c}\binom{\beta}{a}(-1)^{a+\alpha-c}\right).$$

We are now going to investigate the sum. First notice that we can substitute α with i and β with $2n-1-i$ to obtain

$$\sum_{i=0}^{n-1}\left(\binom{2n}{i+1} - \binom{2n}{i} + (-1)^i\right)(-1)^{a-c+i+1}\left(\binom{i}{a}\binom{2n-1-i}{c} + \binom{i}{c}\binom{2n-1-i}{a}\right). \quad (5)$$

Now if we apply the substitution $i \mapsto 2n-1-j$ we obtain

$$\sum_{j=n}^{2n-1}\left(\binom{2n}{j+1} - \binom{2n}{j} + (-1)^j\right)(-1)^{a-c+j+1}\left(\binom{j}{a}\binom{2n-1-j}{c} + \binom{j}{c}\binom{2n-1-j}{a}\right)$$

and thus we have that equation (5) equals

$$\frac{1}{2}\sum_{i=0}^{2n-1}\left(\binom{2n}{i+1} - \binom{2n}{i} + (-1)^i\right)(-1)^{a-c+i+1}\Bigg(\underbrace{\binom{i}{a}\binom{2n-1-i}{c}}_{(I)} + \underbrace{\binom{i}{c}\binom{2n-1-i}{a}}_{(II)}\Bigg) \quad (6)$$

where importantly we now sum to $2n-1$. Observe now that (I) vanishes if not $a \le i \le a+b$ and (II) vanishes if not $c \le i \le b+c$. Thus, we can split the sum in the part containing (I) summing from a to $a+b$ and the part containing (II) summing from c to $b+c$. Moreover, we apply the substitution $i \mapsto a+j$ to the first and $i \mapsto b+c-j$ to the second sum to obtain:

$$\frac{1}{2}(-1)^{a-c}\sum_{j=0}^{b}\left(\binom{2n}{a+j+1} - \binom{2n}{a+j} + (-1)^{a+j}\right)(-1)^{a+j+1}\binom{a+j}{a}\binom{b+c-j}{c}$$
$$+\frac{1}{2}(-1)^{a-c}\sum_{j=0}^{b}\left(\binom{2n}{b+c+j+1} - \binom{2n}{b+c+j} + (-1)^{b+c-j}\right)(-1)^{b+c-j+1}\binom{b+c-j}{c}\binom{a-j}{a}.$$

Using that $b+c = 2n-1-a$ we find that the second sum equals the first and thus that (6) can be written as

$$(-1)^{a-c}\sum_{j=0}^{b}\Bigg(\underbrace{\binom{2n}{a+j+1}}_{(I)}-\underbrace{\binom{2n}{a+j}}_{(II)}+\underbrace{(-1)^{a+j}}_{(III)}\Bigg)(-1)^{a+j+1}\binom{a+j}{a}\binom{b+c-j}{c}.$$

Now we can consider the three parts $(I),(II),(III)$ of the sum separately. We find for (II):

$$\begin{aligned}(-1)^{c}\sum_{i=0}^{b}(-1)^{i}\binom{2n}{a+i}\binom{a+i}{a}\binom{b+c-i}{c}&=(-1)^{c}\binom{2n}{a}\sum_{i=0}^{b+c}(-1)^{i}\binom{b+c+1}{i}\binom{b+c-i}{c}\\&=(-1)^{c}\binom{2n}{a}\binom{-1}{b}=(-1)^{b+c}\binom{2n}{a}=(-1)^{a+1}\binom{2n}{a},\end{aligned}$$

where in the first equality we used the first identity from Lemma 1.3 with $\overline{n}=2n$, $\overline{k}=i$ and $\overline{h}=a$, the fact that $2n-a=b+c+1$ as well as that the sum vanishes for $i>b$. In the second equality we used the second identity from Lemma 1.3 with $\overline{r}=b+c$, $\overline{k}=i$, $\overline{t}=0$, $\overline{m}=c$ and $\overline{s}=b+c+1$. In the third equality we used the fifth identity from Lemma 1.3 and finally in the fourth equality we again used that $b+c=2n-a-1$.

For (I) notice that by applying the substitution $i\mapsto b-j$ we get

$$(-1)^{a}\sum_{j=0}^{b}(-1)^{j}\binom{2n}{c+j}\binom{c+j}{c}\binom{a+b-j}{a}=(-1)^{c+1}\binom{2n}{c}$$

where we observed that the expression on the left is the same as the one for (I) just with a and c exchanged and thus we get the result on the right.

Finally for (II) we have:

$$(-1)^{a+c+1}\sum_{i=0}^{b}\binom{a+i}{a}\binom{b+c-i}{c}=(-1)^{b}\binom{2n}{b}$$

where we used the sixth identity from Lemma 1.3 with $\overline{n}=a$, $\overline{m}=c$, $\overline{r}=b+c$ and $\overline{s}=a$ as well as that $a+c+1=2n-b$. Combining all the above we get the desired result. □

Notice that the above result gives precisely the same as Theorem 2.14. This shows Theorem 2.13 by example for the case of odd depth 2 words. Similarly, we can find an expression for the single-valued MZVs of even depth 2 words. Let $w=x^{a}yx^{b}yx^{c}$ of even length $2n$. Then the only terms in τ^{t} that can give w are

$$I_{1}^{l}c_{2l}\operatorname{ad}_{x}^{2l}(y)\circ(I_{m}^{1}c_{2m}\operatorname{ad}_{x}^{2m}(y)\circ 1)$$

where $\circ$ denotes the action from Definition 2.25 and $l+m=n-1$ Expanding this and plugging in the definition for c_{2n} we get

$$\begin{aligned}4\frac{\zeta(2l+1)\zeta(2m+1)}{(2\pi i)^{2n}}\sum_{i=1}^{l}\sum_{j=1}^{m}\binom{2l}{i}\binom{2m}{j}(-1)^{i+j}\Big(&x^{i}yx^{2l-i+j}yx^{2m-j}+x^{j}yx^{i}yx^{2l+2m-i-j}\\&-x^{i+j}yx^{2l-i}yx^{2m-j}\Big)\end{aligned}$$

we then find that the first term contributes w if $i=a$ and $j=2m-c$. The second term contributes if $i=b$ and $j=a$ and the third term contributes if $i=2l-b$ and $j=2m-c$. In total this gives that the coefficient of w in τ^t (up to the $(t(1-t))^{2n}$) is given by

$$4\sum_{l+m=n-1}\left((-1)^{a+c}\binom{2l}{a}\binom{2m}{c}+(-1)^{a+b}\binom{2l}{b}\binom{2m}{a}-(-1)^{b+c}\binom{2l}{b}\binom{2m}{c}\right)\frac{\zeta(2l+1)\zeta(2m+1)}{(2\pi i)^{2n}}.$$

This proves Theorem 2.15.

3.2 The depth 3 coefficients $c_{\alpha,\beta,\gamma}$

Let us now turn to the coefficients in depth 3. First we need to find a basis of $\mathbb{F}_{\mathrm{Lie}}(x,y)$ in depth 3. For this we need the definition of a Lyndon word:

Definition 3.8. Let X be a totally ordered alphabet. Then a word w in X is called *Lyndon word* if w is the unique minimal element in the lexicographical ordering of the set of all rotations of w.

A general known fact is, that for $\mathbb{F}_{\mathrm{Lie}}(X)$, the free Lie algebra with generating set X, there exists a bijection γ between the Lyndon words in X and a basis of $\mathbb{F}_{\mathrm{Lie}}(X)$. The bijection is given as follows:

- If $|w|=1$ then $\sigma(w)=w$.
- If $|w|>1$ then write $w=uv$ for u and v Lyndon words and with v having maximal length. Then $\gamma(w)=[\gamma(u),\gamma(v)]$.

We are going to use this bijection to find a basis of $\mathbb{F}_{\mathrm{Lie}}(x,y)$ in depth 3. The Lyndon words of depth 3 are given by $w=yx^{\alpha}yx^{\beta}yx^{\gamma}$ with $\alpha\leq\beta$, $\alpha<\gamma$. As, if $\alpha=\gamma$ we distinguish:

- If $\beta=\alpha$ then w is not a Lyndon word as there exist no unique minimal rotation of w.
- If $\beta<\alpha$ then $yx^{\gamma}yx^{\alpha}yx^{\beta}$ would be smaller than w.

The image of w under γ is given as

$$\gamma(w)=\begin{cases}\left[\mathrm{ad}_x^{\alpha}(y),\left[\mathrm{ad}_x^{\beta}(y),\mathrm{ad}_x^{\gamma}(y)\right]\right] & \text{for } \beta<\gamma\\ \left[\left[\mathrm{ad}_x^{\alpha}(y),\mathrm{ad}_x^{\beta}(y)\right],\mathrm{ad}_x^{\gamma}(y)\right] & \text{for } \beta\geq\gamma\end{cases}.$$

Notice that the second term can be rearranged as follows:

$$\begin{aligned}&\left[\left[\mathrm{ad}_x^{\alpha}(y),\mathrm{ad}_x^{\beta}(y)\right],\mathrm{ad}_x^{\gamma}(y)\right] \quad \text{for} \quad \alpha<\gamma\leq\beta\\ =&-\left[\mathrm{ad}_x^{\gamma}(y),\left[\mathrm{ad}_x^{\alpha}(y),\mathrm{ad}_x^{\beta}(y)\right]\right] \quad \text{for} \quad \alpha<\gamma\leq\beta\\ =&-\left[\mathrm{ad}_x^{\alpha'}(y),\left[\mathrm{ad}_x^{\beta'}(y),\mathrm{ad}_x^{\gamma'}(y)\right]\right] \quad \text{for} \quad \beta'<\alpha'\leq\gamma'\end{aligned}$$

where in the last step we used the substitution $\alpha'=\gamma$, $\beta'=\alpha$ and $\gamma'=\beta$. Combining this we find that a basis in depth 3 can be given by

$$\left\{\left[\mathrm{ad}_x^{\alpha}(y),\left[\mathrm{ad}_x^{\beta}(y),\mathrm{ad}_x^{\gamma}(y)\right]\right]\right\}_{\beta<\gamma,\alpha\leq\gamma}.$$

Let us now fix $n\geq 1$ and consider $\tau_{2n+1}\in\widehat{\mathbb{F}}_{\mathrm{Lie}}(x,y)_{2n+1}$ (the linear span of Lie words in 2n brackets). Using the above basis, we may write τ_{2n+1} in depth 3 as follows,

$$\tau_{2n+1}=\sum_{\substack{\beta<\gamma,\alpha\leq\gamma\\ \alpha+\beta+\gamma=2n-2}}c_{\alpha,\beta,\gamma}\left[\mathrm{ad}_x^{\alpha}(y),\left[\mathrm{ad}_x^{\beta}(y),\mathrm{ad}_x^{\gamma}(y)\right]\right]$$

The value for $\alpha+\beta+\gamma$ follows as every $\mathrm{ad}_x^k(y)$ contains k Lie brackets and then bracketing together the $\mathrm{ad}_x^k(y)$ terms uses another 2 brackets. With this shown we can now come back to the defining equation (2) and only consider the terms that could give the word $w = x^a y x^b y x^c y x^d$ where w is of length $2n+1$. We get the following:

$$-u_w w = \left(1 + \sum_{s\in\mathbb{N}} I_1^s \tau_{2s+1} + \sum_{l,m\in\mathbb{N}} J_1^{l,m} \tau_{2l+1}\tau_{2m+1} + \sum_{l,m,h\in\mathbb{N}} K_1^{l,m,h} \tau_{2l+1}(\tau_{2m+1}\tau_{2h+1}) + \dots\right)$$
$$\circ \left(1 + u_w w + \sum_{p,q,r\in\mathbb{N}_0} u_{x^p y x^q y x^r} x^p y x^q y x^r + \sum_{p,q\in\mathbb{N}_0} u_{x^p y x^q} x^p y x^q + \dots\right) \tag{7}$$

Let us now expand the right hand side. The action of 1 on Φ_{KZ} only gives $u_w w$. From the action of the single integrals $\sum_{s\in\mathbb{N}} I_1^s \tau_{2s+1}$ on Φ_{KZ} we get

$$\sum_{\substack{\beta<\gamma,\alpha\leq\gamma\\ \alpha+\beta+\gamma+3=|w|}} I_1^{|w|-1} c_{\alpha,\beta,\gamma} \left[\mathrm{ad}_x^\alpha(y), \left[\mathrm{ad}_x^\beta(y), \mathrm{ad}_x^\gamma(y)\right]\right] \circ 1$$
$$+ \sum_{\substack{s\in\mathbb{N},0\leq\alpha<\beta\\ \alpha+\beta=2s-1}} I_1^s c_{\alpha,\beta} \left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right] \circ \sum_{p,q\in\mathbb{N}_0} u_{x^p y x^q} x^p y x^q$$
$$+ \sum_{s\in\mathbb{N}} I_1^s c_{2s} \,\mathrm{ad}_x^{2s}(y) \circ \sum_{p,q,r\in\mathbb{N}_0} u_{x^p y x^q y x^r} x^p y x^q y x^r.$$

Importantly, here the first term only contributes if $|w|$ is odd as the τ_{2j} and thus also the $c_{\alpha,\beta,\gamma}$ for $\alpha+\beta+\gamma+3$ even are 0. Considering the action of the double integrals $\sum_{l,m\in\mathbb{N}} J_1^{l,m} \tau_{2l+1}\tau_{2m+1}$ on Φ_{KZ} we obtain

$$\sum_{l,m\in\mathbb{N}} J_1^{l,m} c_{2l} c_{2m} \,\mathrm{ad}_x^{2l} \circ (\mathrm{ad}_x^{2m} \circ x^p y x^q) u_{x^p y x^q}$$
$$+ \sum_{l,m\in\mathbb{N}} \sum_{\substack{0\leq\alpha<\beta\\ \alpha+\beta=2l-1}} J_1^{l,m} c_{\alpha,\beta} c_{2m} \left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right] \circ \left(\mathrm{ad}_x^{2m}(y) \circ 1\right)$$
$$+ \sum_{l,m\in\mathbb{N}} \sum_{\substack{0\leq\alpha<\beta\\ \alpha+\beta=2m-1}} J_1^{l,m} c_{2l} c_{\alpha,\beta} \,\mathrm{ad}_x^{2l} \circ \left(\left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right] \circ 1\right).$$

Here, the second and third term only contribute in the case of $|w|$ being even, as $[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)]$ is of odd length and so is $\mathrm{ad}_x^{2k}(y)$ thus the action only gives words of even length.
Finally, the action of the triple integrals $\sum_{l,m,h\in\mathbb{N}} K_1^{l,m,h} \tau_{2l+1}(\tau_{2m+1}\tau_{2h+1})$ on Φ_{KZ} gives

$$\sum_{l,m,h\in\mathbb{N}} K_1^{l,m,h} c_{2l} c_{2m} c_{2h} \,\mathrm{ad}_x^{2l}(y) \circ (\mathrm{ad}_x^{2m}(y) \circ (\mathrm{ad}_x^{2h}(y) \circ 1)).$$

In the following we are now going to calculate the exact contribution to a word w for each of these terms which will then give us an equation from which we can calculate the $c_{\alpha,\beta,\gamma}$. To later also calculate the coefficients of the interpolating associators we will do these calculations for arbitrary t and not just $t = 1$.

The $c_{\alpha,\beta,\gamma}$ term

We start with the term

$$\sum_{\substack{\beta<\gamma,\alpha\leq\gamma\\ \alpha+\beta+\gamma=2n-2}} I_t^n c_{\alpha,\beta,\gamma} \left[\mathrm{ad}_x^\alpha(y), \left[\mathrm{ad}_x^\beta(y), \mathrm{ad}_x^\gamma(y)\right]\right] \circ 1$$

and are interested in finding the terms of this sum that give words of the form $w = x^a y x^b y x^c y x^d$ with $a+b+c+d = 2n-2$. From the expansion in Remark 3.2 we find that the coefficient of the word w in the above sum is given by

$$\sum_{\substack{\beta<\gamma,\alpha\leq\gamma\\ \alpha+\beta+\gamma=2n-2}} c_{\alpha,\beta,\gamma}(-1)^{2a+b-d}\left(\binom{\alpha}{a}\binom{\beta}{b+a-\alpha}\binom{\gamma}{d}(-1)^{\gamma-\alpha} - \binom{\alpha}{d}\binom{\beta}{a}\binom{\gamma}{b+a-\beta}(-1)^{\alpha-\beta}\right.$$
$$\left. -\binom{\alpha}{a}\binom{\beta}{d}\binom{\gamma}{b+a-\alpha}(-1)^{\beta-\alpha} + \binom{\alpha}{d}\binom{\beta}{b+a-\gamma}\binom{\gamma}{a}(-1)^{\alpha-\gamma}\right).$$

Our goal is to show that the system of equations for all different a, b, c, d has full rank. For this we are considering the following order on the indices (α, β, γ) with $\alpha + \beta + \gamma = 2n - 2$ Let $(\alpha', \beta', \gamma') < (\alpha, \beta, \gamma)$ if and only if $\gamma' < \gamma$ or $\gamma' = \gamma$ and $\beta' > \beta$. Here, no inequality for $\gamma' = \gamma, \beta' = \beta$ needs to be defined as in this case α', α are already fixed.

Then we can consider the subsystem of the above equations were we set $c = 0$ and $a \leq d, b < d$. By ordering the equations, that is the (a, b, d) and the summands of these equations i.e. the (α, β, γ) by this order in ascending order we can consider the matrix of these coefficients. Let us denote it by M, i.e.

$$m_{(a,b,d)(\alpha,\beta,\gamma))} = (-1)^{2a+b-d}\left(\binom{\alpha}{a}\binom{\beta}{b+a-\alpha}\binom{\gamma}{d}(-1)^{\gamma-\alpha} - \binom{\alpha}{d}\binom{\beta}{a}\binom{\gamma}{b+a-\beta}(-1)^{\alpha-\beta}\right.$$
$$\left. -\binom{\alpha}{a}\binom{\beta}{d}\binom{\gamma}{b+a-\alpha}(-1)^{\beta-\alpha} + \binom{\alpha}{d}\binom{\beta}{b+a-\gamma}\binom{\gamma}{a}(-1)^{\alpha-\gamma}\right)$$

with $a \leq d, b < d$ and $\beta < \gamma, \alpha \leq \gamma$.

Theorem 3.9. *The above defined matrix M is in row echelon form with non-zero entries on the diagonal. In particular M is of full rank.*

Proof. Assume a, b, d with $a + b + d = 2n - 2$ and $a \leq c, b < d$. Then let $(\alpha, \beta, \gamma) < (a, b, d)$. If $\gamma < d$ notice that as $\alpha \leq \gamma < d$ and $\beta < \gamma < d$ we have $\binom{\gamma}{d} = \binom{\alpha}{d} = \binom{\beta}{d} = 0$. Contrary if $\gamma = d$ we have $\beta > b$ and then $\alpha = 2n - 2 - \gamma - \beta < m - d - b = a$ from which $\alpha < a \leq d$ follows. Thus, $\binom{\alpha}{a} = \binom{\alpha}{d} = 0$. In both cases all four terms in $m_{(a,b,d)(\alpha,\beta,\gamma)}$ are 0 and thus $m_{(a,b,d)(\alpha,\beta,\gamma)}$ vanishes. We therefore have that M is in row echelon form. It remains to show that the diagonal entries are non-zero.

If $(\alpha, \beta, \gamma) = (a, b, d)$ we distinguish $a < d$ and $a = d$. If $a < d$ then $\binom{\alpha}{d} = \binom{\beta}{d} = 0$ and thus the second, third and fourth term in $m_{(a,b,d)(\alpha,\beta,\gamma)}$ are 0. In the first term however all binomial coefficients are one and thus $m_{(a,b,d)(\alpha,\beta,\gamma)} = (-1)^{2a+b+\gamma-\alpha}$. If however $a = d$ then $\binom{\beta}{a} = \binom{\beta}{d} = 0$ and thus the second and third terms vanish. The first and fourth term are then equal and all binomial coefficients equal 1. Thus, $m_{(a,b,d)(\alpha,\beta,\gamma)} = 2 \cdot (-1)^{2a+b}$ and we conclude the proof. □

From this theorem it follows that by solving the system of linear equations we can fully recover the $c_{\alpha,\beta,\gamma}$.

The remaining terms

The following lemmata cover the remaining terms. Proofs of these can be found in Section 5.

Lemma 3.10. *Let $a,b,c,d \in \mathbb{N}_0$ then the contribution of the word $x^ayx^byx^cyx^d$ by the term*

$$\Delta^t_{single}(w) := \sum_{\substack{s\in\mathbb{N}, 0\le\alpha<\beta \\ \alpha+\beta=2s-1}} I^s_t c_{\alpha,\beta}\left[\mathrm{ad}^\alpha_x(y), \mathrm{ad}^\beta_x(y)\right] \circ \sum_{p,q\in\mathbb{N}_0} u_{x^pyx^q} x^pyx^q$$
$$+ \sum_{s\in\mathbb{N}} I^s_t c_{2s}\,\mathrm{ad}^{2s}_x(y) \circ \sum_{p,q,r\in\mathbb{N}_0} u_{x^pyx^qyx^r} x^pyx^qyx^r.$$

is given by

$$\sum_{\substack{s\in\mathbb{N},p\in\mathbb{N}_0 \\ \alpha+\beta=2s-1 \\ 2s-1=a+b+c-p}} c_{\alpha,\beta} I^s_t \left(\binom{\alpha}{a}\binom{\beta}{b+a-\alpha}(-1)^{2a+b-\alpha} - \binom{\alpha}{b+a-\beta}\binom{\beta}{a}(-1)^{2a+b-\beta}\right.$$
$$\left.+\binom{\alpha}{b+c-\beta}\binom{\beta}{c}(-1)^{2c+b-\beta} - \binom{\alpha}{c}\binom{\beta}{b+c-\alpha}(-1)^{2c+b-\alpha}\right) u_{x^pyx^d}$$
$$+ \sum_{\substack{s\in\mathbb{N},q\in\mathbb{N}_0 \\ \alpha+\beta=2s-1 \\ 2s-1=d+b+c-q}} c_{\alpha,\beta} I^s_t \left(\binom{\alpha}{b}\binom{\beta}{b+c-\alpha}(-1)^{2b+c-\alpha} - \binom{\alpha}{b+c-\beta}\binom{\beta}{b}(-1)^{2b+c-\beta}\right) u_{x^ayx^q}$$
$$+ \sum_{2s=a+b-p} I^{2s}_1 c_{2s}\left(\binom{2s}{a}(-1)^a - \binom{2s}{b}(-1)^b\right) u_{x^pyx^cyx^d} + \sum_{2s=c+d-r} I^{2s}_1 c_{2s}\binom{2s}{c}(-1)^c u_{x^ayx^byx^r}$$
$$+ \sum_{2s=b+c-q} I^{2s}_1 c_{2s}\left(\binom{2s}{b}(-1)^b - \binom{2s}{c}(-1)^c\right) u_{x^ayx^qyx^d}$$

Lemma 3.11. *Let $a,b,c,d \in \mathbb{N}_0$ then the contribution of the word $x^ayx^byx^cyx^d$ by the term*

$$\Delta^t_{double}(w) := \sum_{l,m\in\mathbb{N}} J^{l,m}_t c_{2l}c_{2m}\,\mathrm{ad}^{2l}_x \circ(\mathrm{ad}^{2m}_x \circ x^pyx^q) u_{x^pyx^q}$$

is given by

$$\sum_{\substack{l,m\in\mathbb{N},p\in\mathbb{N}_0 \\ p=a+b+c-2l-2m}} J^{l,m}_t c_{2l}c_{2m}\left(\binom{2l}{a}\binom{2m}{a+b-2l}(-1)^b - \binom{2l}{a}\binom{2m}{c}(-1)^{a-c} + \binom{2l}{b}\binom{2m}{a}(-1)^{a+b}\right.$$
$$- \binom{2l}{b}\binom{2m}{a+b-2l}(-1)^a - \binom{2l}{c}\binom{2m}{a}(-1)^{a-c} - \binom{2l}{b}\binom{2m}{b+c-2l}(-1)^c$$
$$\left.+\binom{2l}{b}\binom{2m}{c}(-1)^{b+c} + \binom{2l}{c}\binom{2m}{b+c-2l}(-1)^b\right) u_{x^pyx^d}$$
$$+ \sum_{\substack{l,m\in\mathbb{N},q\in\mathbb{N}_0 \\ q=b+c+d-2l-2m}} J^{l,m}_t c_{2l}c_{2m}\left(\binom{2l}{b}\binom{2m}{b+c-2l}(-1)^c\right.$$
$$\left.+\binom{2l}{c}\binom{2m}{b}(-1)^{b+c} - \binom{2l}{c}\binom{2m}{b+c-2l}(-1)^b\right) u_{x^ayx^q}$$
$$+2\cdot \sum_{\substack{l,m\in\mathbb{N},p,q\in\mathbb{N}_0 \\ p=a+b-2m \\ q=c+d-2l}} J^{l,m}_t c_{2l}c_{2m}\left(\binom{2l}{c}\binom{2m}{a}(-1)^{a+c} - \binom{2l}{c}\binom{2m}{b}(-1)^{c-b}\right) u_{x^pyx^q}.$$

Lemma 3.12. *Let $a,b,c,d \in \mathbb{N}_0$ then the contribution of the word $x^ayx^byx^cyx^d$ for $a+b+c+$*

$d+3=2n$ by the term

$$\Delta^t_{double\ even}(w) := \sum_{l,m\in\mathbb{N}} \sum_{\substack{0\le\alpha<\beta\\ \alpha+\beta=2l-1}} J_t^{l,m} c_{\alpha,\beta} c_{2m} \left[\operatorname{ad}_x^{\alpha}(y), \operatorname{ad}_x^{\beta}(y)\right] \circ \left(\operatorname{ad}_x^{2m}(y)\circ 1\right)$$

$$+ \sum_{l,m\in\mathbb{N}} \sum_{\substack{0\le\alpha<\beta\\ \alpha+\beta=2m-1}} J_t^{l,m} c_{2l} c_{\alpha,\beta} \operatorname{ad}_x^{2l} \circ \left(\left[\operatorname{ad}_x^{\alpha}(y), \operatorname{ad}_x^{\beta}(y)\right]\circ 1\right)$$

is given by

$$\sum_{\substack{2l+2m=2n-3\\ \alpha+\beta=2l}} J_t^{l,m} c_{\alpha,\beta} c_{2m} \Bigg(\binom{\alpha}{a}\binom{\beta}{a+b-\alpha}\binom{2m}{d}(-1)^{b+d-\alpha} - \binom{\alpha}{a+b-\beta}\binom{\beta}{a}\binom{2m}{d}(-1)^{b+d-\beta}$$

$$+\binom{\alpha}{b}\binom{\beta}{b+c-\alpha}\binom{2m}{a}(-1)^{a+c-\alpha} - \binom{\alpha}{a+d-2m}\binom{\beta}{c}\binom{2m}{d}(-1)^{a+c-\beta}$$

$$-\binom{\alpha}{b+c-\beta}\binom{\beta}{b}\binom{2m}{a}(-1)^{a+c-\beta} + \binom{\alpha}{c}\binom{\beta}{a+d-2m}\binom{2m}{d}(-1)^{a+c-\alpha}\Bigg)$$

$$+ \sum_{\substack{2l+2m=2n-3\\ \alpha+\beta=2m}} J_t^{l,m} c_{2l} c_{\alpha,\beta} \Bigg(\binom{\alpha}{a+b-2l}\binom{\beta}{d}\binom{2l}{a}(-1)^{b+d-,\beta} - \binom{\alpha}{d}\binom{\beta}{a+b-2l}\binom{2l}{a}(-1)^{b+d-\alpha}$$

$$\binom{\alpha}{a}\binom{\beta}{d}\binom{2l}{b}(-1)^{a+b+d-\beta} - \binom{\alpha}{a+b-2l}\binom{\beta}{d}\binom{2l}{b}(-1)^{a+d-\beta}$$

$$+\binom{\alpha}{a}\binom{\beta}{a+b-\alpha}\binom{2l}{c}(-1)^{b+c-\alpha} - \binom{\alpha}{a}\binom{\beta}{d}\binom{2l}{c}(-1)^{a+c+d-\beta}$$

$$-\binom{\alpha}{d}\binom{\beta}{a}\binom{2l}{b}(-1)^{a+b+d-\alpha} + \binom{\alpha}{d}\binom{\beta}{a+b-2l}\binom{2l}{b}(-1)^{a+d-\alpha}$$

$$-\binom{\alpha}{a+b-\beta}\binom{\beta}{a}\binom{2l}{c}(-1)^{b+c-\beta} + \binom{\alpha}{d}\binom{\beta}{a}\binom{2l}{c}(-1)^{a+c+d-\alpha}\Bigg).$$

Lemma 3.13. *Let $a,b,c,d\in\mathbb{N}_0$ then the contribution of the word $w=x^ayx^byx^cyx^d$ for $a+b+c+d+3=2n+1$ by the term*

$$\Delta^t_{triple}(w) := \sum_{l,m,h\in\mathbb{N}} K_t^{l,m,h} c_{2l}c_{2m}c_{2h} \operatorname{ad}_x^{2l}(y)\circ(\operatorname{ad}_x^{2m}(y)\circ(\operatorname{ad}_x^{2h}(y)\circ 1))$$

is given by

$$\sum_{l+m+h=n-1} K_t^{l,m,h} c_{2l}c_{2m}c_{2h} \Bigg(\binom{2l}{a}\binom{2m}{a+b-2l}\binom{2h}{d}(-1)^{b-d} + \binom{2l}{a}\binom{2m}{c}\binom{2h}{a+b-2l}(-1)^{b+c}$$

$$-\binom{2l}{a}\binom{2m}{c}\binom{2h}{d}(-1)^{a-c-d} + \binom{2l}{b}\binom{2m}{a}\binom{2h}{d}(-1)^{a+b-d}$$

$$-\binom{2l}{b}\binom{2m}{a+b-2l}\binom{2h}{d}(-1)^{a-d} + \binom{2l}{c}\binom{2m}{a}\binom{2h}{a+b-2m}(-1)^{b+c}$$

$$-\binom{2l}{c}\binom{2m}{a}\binom{2h}{d}(-1)^{a-c-d} + \binom{2l}{b}\binom{2m}{b+c-2l}\binom{2h}{a}(-1)^{a+c}$$

$$-\binom{2l}{b}\binom{2m}{c}\binom{2h}{a+b-2l}(-1)^{a+c} + \binom{2l}{c}\binom{2m}{b}\binom{2h}{a}(-1)^{a+b+c}$$

$$
\begin{aligned}
&-\binom{2l}{c}\binom{2m}{b+c-2l}\binom{2h}{a}(-1)^{a+b}-\binom{2l}{b}\binom{2m}{a+d-2h}\binom{2h}{d}(-1)^{a+b}\\
&+\binom{2l}{b}\binom{2m}{c}\binom{2h}{d}(-1)^{b+c+d}-\binom{2l}{c}\binom{2m}{b}\binom{2h}{a+b-2m}(-1)^{a+c}\\
&+\binom{2l}{c}\binom{2m}{a+d-2h}\binom{2h}{d}(-1)^{a-c}\Bigg).
\end{aligned}
$$

Finally, we can turn back to calculating the $c_{\alpha,\beta,\gamma}$. From equation (7) we get the following system of equations

$$
\sum_{\substack{\beta<\gamma,\alpha\leq\gamma\\ \alpha+\beta+\gamma=2n-2}} I_t^n c_{\alpha,\beta,\gamma} m_{(a,b,d)(\alpha,\beta,\gamma)} = -2\cdot u_v - \Delta^1_{single}(v) - \Delta^1_{double}(v) - \Delta^1_{triple}(v)
$$

where $v = x^a y x^b y^2 x^d$ which as shown above has a unique solution. This has been implemented in Python as described in Appendix C. The results for the coefficients of depth 3 for small n can be found in Appendix D.

3.3 The interpolating associators in depth 3

To calculate the values of the associator

$$
\Phi^t = \mathcal{P}\exp\left(\int_0^t \tau^s\, \mathrm{d}s\right)\cdot \Phi_{KZ}
$$

in depth 3 we can use the right hand side of equation (7) where we replace the integrals $I_1^s, J_1^{l,m}, K_1^{l,m,h}$ by $I_t^s, J_t^{l,m}, K_t^{l,m,h}$. Distinguishing then between words of odd and even length we get the following formulae:

Theorem 3.14. *Let $w = x^a y x^b y x^c y x^d$ then for $|w| = 2n+1$,*

$$
\Phi^t(w) = u_w + \sum_{\substack{\beta<\gamma,\alpha\leq\gamma\\ \alpha+\beta+\gamma=2n-2}} I_t^n c_{\alpha,\beta,\gamma} m_{(a,b,d)(\alpha,\beta,\gamma)} + \Delta^t_{single}(w) + \Delta^t_{double}(w) + \Delta^t_{triple}(w)
$$

and for $|w| = 2n$,

$$
\Phi^t(w) = u_w + \Delta^t_{single}(w) + \Delta^t_{double}(w) + \Delta^t_{double\ even}(w).
$$

Importantly, for the case of $t = 1/2$ we get the Alekseev-Torossian associator. In this case we make the following observation:

Theorem 3.15. *Let $w = x^{k_1} y \dots y x^{k_n}$. Then if $|w|$ is odd $\Phi_{AT}(w) = 0$, that is Φ_{AT} vanishes on odd words.*

Proof. The associator Φ_{AT} can be written in two ways

$$
\Phi_{AT} = \mathcal{P}\exp\left(\int_0^{\frac{1}{2}} \tau^t\, \mathrm{d}t\right)\circ\Phi_{KZ} \quad \text{and} \quad \Phi_{AT} = \mathcal{P}\exp\left(\int_1^{\frac{1}{2}} \tau^t\, \mathrm{d}t\right)\circ\Phi_{\overline{KZ}}
$$

where the second one follows by traversing the path from Φ_{KZ} to $\Phi_{\overline{KZ}}$ in the other direction. Notice that τ^t is invariant under the substitution $t \mapsto (1-t)$ as t always appears as $(t(t-1))^{2i}$.

We can now transform the integrals in $\mathcal{P}\exp\left(\int_1^{\frac{1}{2}} \tau^t \,\mathrm{d}t\right)$ as follows

$$\int_1^{\frac{1}{2}} \int_1^{t_1} \cdots \int_1^{t_{n-1}} \tau^{t_1} \circ \ldots \circ \tau^{t_n} \,\mathrm{d}t_n \ldots \mathrm{d}t_1 = \int_0^{\frac{1}{2}} \int_0^{t_1} \cdots \int_0^{t_{n-1}} (-1)^n \tau^{t_1} \circ \ldots \circ \tau^{t_n} \,\mathrm{d}t_n \ldots \mathrm{d}t_1$$

where we used the above discussed substitution and the $(-1)^n$ comes from substituting the $\mathrm{d}t_i$. If we apply this transformation to the whole time-ordered exponential we get:

$$\mathcal{P}\exp\left(\int_1^{\frac{1}{2}} \tau^t \,\mathrm{d}t\right) = \mathcal{P}\exp\left(\int_0^{\frac{1}{2}} (-\tau^t) \,\mathrm{d}t\right).$$

Let us denote the inversion map $(x, y) \mapsto (-x, -y)$ by Θ. Then we find:

$$\begin{aligned} \Phi_{AT} &= \mathcal{P}\exp\left(\int_0^{\frac{1}{2}} \tau^t \,\mathrm{d}t\right) \circ \Phi_{KZ} \\ &= \left(\mathcal{P}\exp\left(\int_0^{\frac{1}{2}} -\tau^t \,\mathrm{d}t\right) \Phi_{\overline{KZ}}\right) \circ \Theta \\ &= \left(\mathcal{P}\exp\left(\int_1^{\frac{1}{2}} \tau^t \,\mathrm{d}t\right) \circ \Phi_{\overline{KZ}}\right) \circ \Theta = \Phi_{AT} \circ \Theta \end{aligned}$$

where in the second equality we used the fact that in τ^t only odd words appear and thus applying Θ to those words gives a minus. Rewriting this for a specific word w gives

$$\Phi_{AT}(w) = (-1)^{|w|} \Phi_{AT}(w)$$

from which the desired statement follows. □

Remark 3.16. Let w be a word of depth n. Notice that the above proposition shows that to $\Phi_{AT}(w)$ in depth n only terms of $\tau^{1/2}$ of depth $n-1$ contribute.

The calculation of these coefficients has also been realized in the Python implementation described in Appendix C.

Example 3.17. For words of length 4 and 6 we find the following coefficients of AT:

$$\Phi_{AT}(y^2x^1y) = -\frac{1}{480} \qquad \Phi_{AT}(y^3x^1) = \frac{1}{1440} \qquad \Phi_{AT}(yx^1y^2) = \frac{1}{480} \qquad \Phi_{AT}(x^1y^3) = -\frac{1}{1440}$$

as well as

$$\begin{aligned}
&\Phi_{AT}(y^2x^3y) = \frac{89}{2903040} && \Phi_{AT}(y^2x^2yx^1) = -\frac{17}{580608} && \Phi_{AT}(y^2x^1yx^2) = \frac{29}{414720} \\
&\Phi_{AT}(y^3x^3) = -\frac{23}{967680} && \Phi_{AT}(yx^1yx^2y) = -\frac{143}{2903040} && \Phi_{AT}(yx^1yx^1yx^1) = -\frac{31}{967680} \\
&\Phi_{AT}(yx^1y^2x^2) = -\frac{17}{580608} && \Phi_{AT}(yx^2yx^1y) = \frac{37}{580608} && \Phi_{AT}(yx^2y^2x^1) = \frac{13}{967680} \\
&\Phi_{AT}(yx^3y^2) = -\frac{11}{290304} && \Phi_{AT}(x^1y^2x^2y) = -\frac{13}{967680} && \Phi_{AT}(x^1y^2x^1yx^1) = -\frac{143}{2903040} \\
&\Phi_{AT}(x^1y^3x^2) = \frac{89}{2903040} && \Phi_{AT}(x^1yx^1yx^1y) = \frac{1}{322560} && \Phi_{AT}(x^1yx^1y^2x^1) = \frac{37}{580608} \\
&\Phi_{AT}(x^1yx^2y^2) = \frac{53}{1451520} && \Phi_{AT}(x^2y^2x^1y) = \frac{53}{1451520} && \Phi_{AT}(x^2y^3x^1) = -\frac{11}{290304} \\
&\Phi_{AT}(x^2yx^1y^2) = -\frac{29}{414720} && \Phi_{AT}(x^3y^3) = \frac{23}{967680}.
\end{aligned}$$

Remark 3.18. Even though these results might suggest that Φ_{AT} is anti-symmetric under the reversal of words this does not hold as can be seen by calculating the coefficient of the word $w = x^4yxy^2$ and $\widetilde{w} = y^2xyx^4$:

$$\Phi_{AT}(x^4yxy^2) = \frac{1133}{180}\frac{\zeta(8)}{(2\pi i)^8} + \frac{7}{10}\frac{\zeta(5,3)}{(2\pi i)^8} + \frac{5943}{4096}\frac{\zeta(5)\zeta(3)}{(2\pi i)^8} + 2\frac{\zeta(2)\zeta(3)^2}{(2\pi i)^8}$$
$$\Phi_{AT}(y^2xyx^4) = -\frac{1133}{180}\frac{\zeta(8)}{(2\pi i)^8} - \frac{7}{10}\frac{\zeta(5,3)}{(2\pi i)^8} - \frac{5943}{4096}\frac{\zeta(5)\zeta(3)}{(2\pi i)^8}.$$

4 The isomorphism from $H^0(\mathsf{GC})$ to $\mathfrak{grt}_1$

In the following section we are going to describe in detail the isomorphism from $H^0(\mathsf{GC})$ to $\mathfrak{grt}_1$ introduced by Willwacher in [22]. In [18] it was shown by Rossi and Willwacher that this isomorphism is induced by a map $\phi : \mathsf{GC} \to \mathfrak{sder}_2$ which we will also discuss. First however, we will describe the different spaces involved. For these sections we follow the descriptions in [20].

Definition 4.1. Let $G = (V, E)$ be a graph. An *ordering* on its edges is a bijective function σ from E to $\{1, \dots, |E|\}$. Notice that $\mathbb{S}_{|E|}$ acts on σ by $\pi \circ \sigma$ for $\pi \in \mathbb{S}_n$. We call the tuple (G, σ) an *ordered graph* and note that $\mathbb{S}_{|E|}$ acts on (G, σ) by $\pi(G, \sigma) = (G, \pi\sigma)$ for $\pi \in \mathbb{S}_{|E|}$. Moreover, we denote by $|e|$ the order number of an edge e.

A map f between two ordered graphs $(G, \sigma) \to (H, \tau)$ is said to be a *ordered graph isomorphism* if f is a graph isomorphism on G, $f(\Phi) = \Psi$ and $\sigma = \tau \circ f$.

In the following we are mostly going to omit the orientation and just write G for (G, σ).

Definition 4.2. A graph is called k-vertex irreducible if after removing any k vertices the graph is still connected.

A simple loop is an edge starting and ending at the same vertex. A graph is called simple if it does not contain any simple loops or multi-edges.

Definition 4.3. For two ordered graphs G, G' a composition $G \circ_j G'$ can be defined by inserting the graph G' at the j-th vertex v_j in G (thereby removing v_j) and then summing over all possible ways to reconnect all edges incident to v_j to vertices in G'. Here in the ordering all edges in G' are placed after the edges in G in the same order they appear in G'.

Example 4.4. Consider the graph G and G' as given in Figure 4 on the left. We then apply the composition $\circ_j$ where j is the vertex in G marked by j to G' which gives the result on the right.

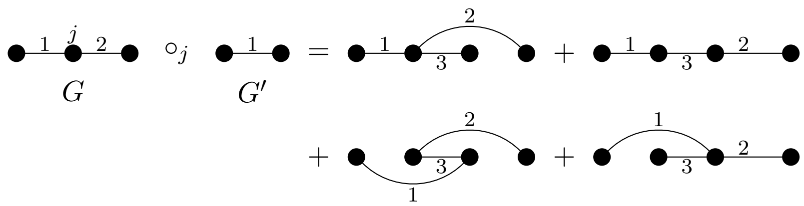


Figure 4: The graph composition of G and G' at the vertex j.

4.1 Kontsevich's graph complex

Definition 4.5. A GC-*admissible graph* G is a loop-less connected ordered graph that is 1-vertex irreducible and every vertex has valency ≥ 3.

We now consider the $\mathbb{Q}$-vector space GC spanned by isomorphism classes of GC-admissible graphs, subject to the relation

$$(G, \pi \circ \sigma) = \operatorname{sgn} \pi \cdot (G, \sigma) \quad \text{for all} \quad \pi \in \mathbb{S}_{|E|}.$$

Under this relation we call σ an *orientation.* Observe that if $(G, \sigma) \simeq (G, \pi \circ \sigma)$ for an odd permutation π then $(G, \sigma) \simeq (G, \pi \circ \sigma) = -(G, \sigma)$ and thus $(G, \sigma) = 0$ in GC.

A grading on GC is given by

$$\deg(G) = 2|V| - |E| - 2.$$

Further, GC carries the structure of a differential graded Lie algebra where the Lie bracket is given by:

$$[G, G'] := G \circ G' - (-1)^{\deg(G)\cdot\deg(G')} G' \circ G.$$

Here $G \circ G'$ is defined as

$$G \circ G' = \sum_{j=1}^{|G|} G \circ_j G'.$$

Finally, we can define a differential on GC as follows:

Definition 4.6. Let $G \in \mathsf{GC}$. Then a differential is given by :

$$d_{\mathsf{GC}} G = [\Gamma_{\bullet\!-\!\bullet}, G] = \Gamma_{\bullet\!-\!\bullet} \circ G - (-1)^{\deg(G)} G \circ \Gamma_{\bullet\!-\!\bullet}.$$

where $\Gamma_{\bullet\!-\!\bullet}$ is the graph given by two vertices connected by an edge. That is the second term of the differential splits every vertex w into two vertices u, v connected by an edge e and then reconnects all the edges incident to w in all possible ways to u and v. Moreover, the new edge e is placed last in the ordering. The first term cancels all the terms of the second where the new vertex is univalent.

For d_{GC} we have that $d_{\mathsf{GC}}^2 = 0$ and thus GC with the differential d_{GC} is a graph complex, called *Kontsevich's graph complex.*

It remains to see that this differential is well-defined.

Lemma 4.7. *The differential* d_{GC} *is well-defined.*

Proof. We need to show that no graphs with bivalent vertices are created by the differential. Let G in GC and let H be a graph occurring in the differential of G. Then H can have at most one bivalent vertex w as G only has vertices with valency ≥ 3 and this vertex needed to be created by the splitting.

This can only occur when a vertex u is being split into u_1, u_2 and all but one edge (call it e) are connected to u_1 / u_2 and the remaining edge e is connected to u_2 / u_1. W.l.o.g. we can assume that w is u_2. Let v be the other vertex of the edge e. i.e. $e = \{u, v\}$. Then the edge going from v to w has the order number $|e|$ and the edge from w to u has the order number $|E(G)| + 1$.

Now this arrangement of edges can also be reached in another way. That is when splitting the vertex v into v_1 and v_2 all edges but e can be connected to v_1 / v_2 and e is connected to v_2 / v_1. Once again we can assume that e is connected to v_2 i.e. v_2 is w. In this case however the edge going from v to w has order number $|E(G)| + 1$ and the edge from w to u has order number $|e|$.

Thus, the two graphs obtained differ by the permutation that permutes $|e|$ and $(|E(G)| + 1)$ and thus cancel. As H was an arbitrary graph with a bivalent vertex all these graphs cancel and $d_{\mathsf{GC}}(G)$ is well-defined.

□

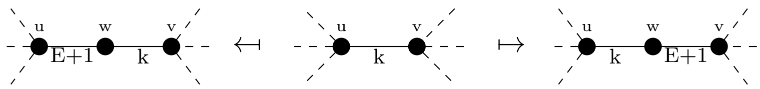


Figure 5: An illustration of the two ways the bivalent vertex w can be created. In the middle the section in the original graph and on the left / right the section where the vertex u / v have been split respectively and all but one edge has been reconnected to one vertex.

4.2 The spaces graphs and ICG

Definition 4.8. A graphs-admissible graph G is an ordered simple graph with labeled vertices $1, \dots, k$, called external, and possibly other vertices, called internal. Moreover, the internal vertices have valency ≥ 3 and for every internal vertex there exists a path in G to an external vertex.

Let us denote the external vertices of G by $V_E(G)$ and the internal vertices by $V_I(G)$. Moreover, in drawings we will draw internal vertices as black dots and external vertices as black circles with white interior.

An isomorphism between external/internal graphs G, H is an ordered graph isomorphism $f : G \to H$ with the extra condition that $f(V_E(G)) = V_E(H)$ and for internal vertices, that f sends the vertex labelled i in G to the vertex labelled i in H. That is external vertices can only be mapped to external ones and internal vertices only to the corresponding internal vertex.

We can consider the $\mathbb{Q}$-vector space $\mathsf{graphs}(k)$ spanned by isomorphism classes of graphs-admissible graphs with k external vertices, subject to the relation

$$(G, \pi \circ \sigma) = \operatorname{sgn} \pi \cdot (G, \sigma) \quad \text{for all} \quad \pi \in \mathbb{S}_{|E|}.$$

The degree on $\mathsf{graphs}(k)$ is given by

$$\deg(G) = |E(G)| - 2|V_I(G)|.$$

Moreover, we can define a differential on $\mathsf{graphs}(k)$ as follows:

Definition 4.9. Let $G \in \mathsf{graphs}(k)$. Then a differential is given by:

$$d_{\mathsf{graphs}} G = \sum_{v \in V_E} G \circ_v \Gamma_{\circ\!-\!\bullet} + \frac{1}{2} \sum_{v \in V_I} G \circ_v \Gamma_{\bullet\!-\!\bullet}$$

where $\Gamma_{\circ\!-\!\bullet}$ is the graph with one internal and one external vertex connected by an edge and $\Gamma_{\bullet\!-\!\bullet}$ is the graph with two internal vertices connected by an edge. That is, the differential splits every external vertex w in one internal u and one external vertex v and connects the edges incident to w in all possible ways to v and u. An internal vertex w is being split into two internal vertices u, v and the edges are once again connected in all possible ways. Moreover, the new edge is placed last in the ordering. Finally, all graphs that result and are not graphs-admissible will be discarded.

The map d_{graphs} as defined above is a differential, that is $d_{\mathsf{graphs}}^2 = 0$ and thus $\mathsf{graphs}(k)$ is a graph complex.

Remark 4.10. Notice that the factor $\frac{1}{2}$ arises as when inserting $\Gamma_{\bullet\!-\!\bullet}$ connecting the edges E_1 to the first vertex and E_2 to the second is the same as connecting the edges E_2 to the first vertex and E_1 to the second. However, when inserting $\Gamma_{\circ\!-\!\bullet}$ into the graph this does not hold as then one vertex is internal and one is external thus they cannot be exchanged and therefore give only half as many summands.

Definition 4.11. We call a graph $G \in \mathsf{graphs}(k)$ internally connected if G is connected after removing all external vertices.

We can then consider the subspace $\mathsf{ICG}(k)$ of $\mathsf{graphs}(k)$ of internally connected graphs with k external vertices. A grading on this space is given by

$$\deg(G) = 2V_I(G) - E(G) + 1.$$

Moreover, $\mathsf{ICG}(k)$ inherits the differential from $\mathsf{graphs}(k)$ by restricting to internally connected graphs. This turns $\mathsf{ICG}(k)$ into a graph complex. Similarly to GC, it also has the structure of a differential graded Lie algebra with the following bracket:

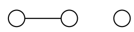
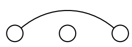
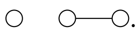
Definition 4.12. The bracket $[G_1, \dots, G_k]$ is given by gluing G_i 's at the corresponding external vertices, then applying the differential of $\mathsf{ICG}(k)$. Here the edges of G_{i+1} are placed after the edges of G_i in the same order they appear in G_{i+1}.

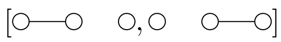
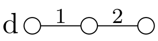
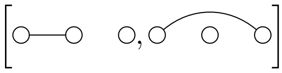
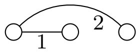
In [20] Severa and Willwacher showed the following important result:

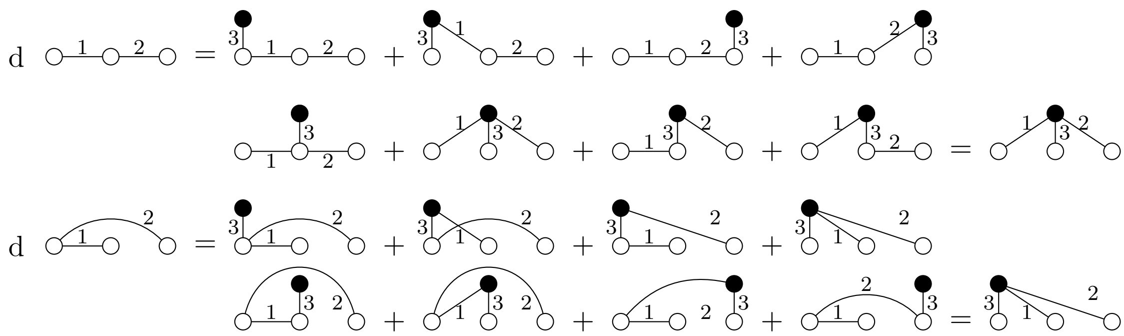
Theorem 4.13. *The cohomology of $\mathsf{ICG}(k)$ is isomorphic to $\mathfrak{t}_k$. Here the isomorphism is given by identifying the generator t_{ij} with the graph consisting of k external and no internal vertices and an edge between the vertex i and j.*

The space $\mathfrak{t}_k$ is the Drinfel'd-Kohno Lie algebra as defined in Definition 2.21. To better understand the Lie bracket on $\mathsf{ICG}(k)$ and the isomorphism we consider the following example:

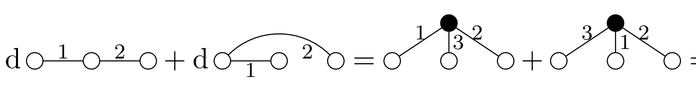
Example 4.14. Consider the space $\mathsf{ICG}(3)$. The goal is to show that the relation $[t_{12}, t_{23} + t_{13}] = 0$ holds for the corresponding graphs in $\mathsf{ICG}(3)$. Notice that we identify these generators as follows:

$t_{12} =$  $t_{13} =$  $t_{23} =$ .

We can then calculate the Lie brackets $[t_{12}, t_{23}] =$  $=$ d  and $[t_{12}, t_{13}] =$  $=$ d  where the differentials give the following:



here we used in the second equality that all non-internally ≥ 3-valent graphs are not graphs-admmissible. We therefore get

$[t_{12}, t_{23} + t_{13}] = [t_{12}, t_{23}] + [t_{12}, t_{13}] =$  $= 0$

where we used that the two last graphs differ by the permutation $(1;3)$ and thus appear with opposite signs.

4.3 The spaces $\mathfrak{tder}_k$ and $\mathfrak{sder}_k$

We denote by $\widehat{\mathbb{F}}_{\text{Lie}}(W)$ the degree completion of the free Lie algebra over $\mathbb{K}$ on the generators W. Let $k := |W|$. Normally, we denote the generators by $x_1, \ldots, x_k$ in the case of $k = 2$ and $k = 3$ we will however denote them by X, Y and X, Y, Z respectively. A grading on $\widehat{\mathbb{F}}_{\text{Lie}}(W)$ can be given by the number of Lie brackets appearing in a Lie monomial. That is, x_i has degree 0, $[x_i, x_j]$ has degree 1, etc.

Definition 4.15. A derivation of a Lie algebra L is a linear map $f : L \to L$ such that

$$f([a, b]) = [f(a), b] + [a, f(b)]$$

for all $a, b \in L$ i.e. the Leibniz rule holds. We denote by $\text{Der}(L)$ the space of all derivations on L. To any element $x, y \in L$ the *inner derivation* $\text{ad}_a(b) := [a, b]$ can be associated. Moreover, the Lie bracket on $\text{Der}(L)$ is given by $[a, b] = a \circ b - b \circ a$, with $a, b \in \text{Der}(L)$ and $\circ$ denoting the composition.

Definition 4.16. On the space $\widehat{\mathbb{F}}_{\text{Lie}}(W)$ a derivation u is called *tangential* if it is of the form

$$u(x_i) = [x_i, u_i]$$

for some $u_i \in \widehat{\mathbb{F}}_{\text{Lie}}(W)$. The space of all tangential derivations on $\widehat{\mathbb{F}}_{\text{Lie}}(W)$ is denoted by $\mathfrak{tder}_k$. Every element u of this space can uniquely be represented by a k-tuple $(u_1, \ldots, u_k)$ with $u_i \in \widehat{\mathbb{F}}_{\text{Lie}}(W)$ such that the term of order 1 with respect to x_i in u_i is 0. This choice of 0 is necessary as the u_i are only defined up to the coefficient of the order 1 term of x_i as $[x_i, x_i] = 0$.

The standard Lie bracket on $\text{Der}(\widehat{\mathbb{F}}_{\text{Lie}}(W))$ induces the following bracket on $\mathfrak{tder}_k$: For the elements $u = (u_1, \ldots, u_k), v = (v_1, \ldots, v_k)$ the bracket is given by

$$[u, v] = (u(v_1) - v(u_1) + [u_1, v_1], \ldots, u(v_k) - v(u_k) + [u_k, v_k])$$

which can be seen as follows

$$\begin{aligned}
[u, v]\,(x_i) &= u(v(x_i)) - v(u(x_i)) = u([x_i, v_i]) - v([x_i, u_i]) \\
&= [u(x_i), v_i] + [x_i, u(v_i)] - [v(x_i), u_i] + [x_i, v(u_i)] \\
&= [[x_i, u_i], v_i] + [x_i, u(v_i)] - [x_i, v(u_i)] - [x_i, [v_i, u_i]] + [v_i, [x_i, u_i]] \\
&= [x_i, u(v_i) - v(u_i) + [u_i, v_i]]
\end{aligned}$$

where for the fourth equality we used the Jacobi identity to get $[[x_i, v_i], u_i] = [x_i, [v_i, u_i]] - [v_i, [x_i, u_i]]$ and in the fifth equality we used the anti-symmetry $[v_i, [x_i, u_i]] = -[[x_i, u_i], v_i]$. Finally, we consider the subspace $\mathfrak{sder}_k \subseteq \mathfrak{tder}_k$ of special derivations, consisting of all tangential derivations satisfying the additional property that

$$u\left(\sum_{i=1}^{k} x_i\right) = \sum_{i=1}^{k} [x_i, u_i] = 0.$$

4.4 Identification between Lie trees and Lie monomials

Elements of the Lie algebra $\widehat{\mathbb{F}}_{\text{Lie}}(W)$ and in particular elements of $\mathfrak{tder}_k$ and $\mathfrak{sder}_k$ admit combinatorial representations via graphs. In the following we are going to discuss those and show some examples. Here we follow [22].

Definition 4.17. Lie monomials in $\widehat{\mathbb{F}}_{\text{Lie}}(W)$ of degree n are associated with directed ordered rooted trees with k external vertices and the further constraint that the root has two outgoing edges, each other internal vertex has two outgoing and one incoming edge and the external vertices only have incoming edges. These trees are being called *Lie trees*.

The correspondence is given as follows: To each external vertex $1, \dots, k$ we associate a generator $x_1, \dots, x_k$ of $\widehat{\mathbb{F}}_{\text{Lie}}(W)$. Then recursively to every internal vertex v with the two outgoing edges $e_1 = (v, w_1)$, $e_2 = (v, w_2)$ such that $e_1 < e_2$ we assign $[L_1, L_2]$ where L_1 and L_2 are the Lie monomials assigned to the vertices w_1 and w_2. This process will finish at the root as it has no incoming edges. Then the monomial associated to the whole tree is the monomial of the root. Moreover, one has to quotient the graded vector space of Lie trees by the IHX-relation (see Figure 6 on the left) to encode the Jacobi-Identity of the Lie bracket.

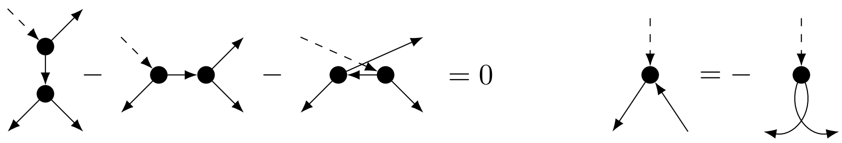


Figure 6: The picture on the left displays the IHX relation and the one on the right shows the anti-symmetry relation. The dashed incoming edges may or may not be present; depending on if this vertex is the root of the Lie tree or not.

Remark 4.18. In some papers Lie trees are defined without the ordering on the edges. Then, however, the sign of the expression is not fixed as for a vertex v it is not clear which outgoing edge corresponds to the first and which to the second argument of the Lie bracket at v. In this case one has to further quotient the space of Lie trees by the anti-symmetry relation shown in Figure 6 on the right.

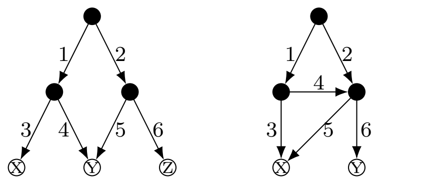


Figure 7: Two Lie trees with their corresponding Lie monomials in $\widehat{\mathbb{F}}_{\text{Lie}}(X, Y, Z)$ and $\widehat{\mathbb{F}}_{\text{Lie}}(X, Y)$ respectively.

Example 4.19. In Figure 7 two examples of Lie Trees with their corresponding polynomials are shown. For the left tree the polynomials associated to the two vertices in the vertical middle are $[X, Y]$ and $[Y, Z]$. For the right tree they are $[X, [X, Y]]$ and $[X, Y]$.

Turning to $\mathfrak{tder}_k$ from the discussion in the previous section we see that its elements are in one-to-one correspondence with k-tuples of Lie trees with k external vertices modulo the IHX relation. However, we can also turn to a more convenient description to encode these k-tuples: For an element $u = (u_1, \dots, u_k) \in \mathfrak{tder}_k$ we consider the linear combination of Lie trees corresponding to u_i. For each of those trees we draw an additional edge from the i-th external vertex to the root. This turns the Lie tree into a directed internally-trivalent graph with k external vertices. As the new edge is the only one leaving an external vertex it uniquely identifies the root as well as the u_j to which it corresponds.

Example 4.20. Consider the tangential derivation given by $u = ([X, Y], [Y, [X, Y]])$. Then its identification with a Lie tree is shown in Figure 8 on the left and its description in terms of the directed internally-trivalent graphs is depicted on the right of Figure 8.

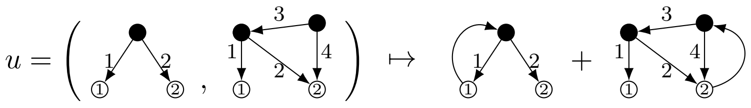


Figure 8: The identification as a Lie tree on the left and as a internally-trivalent directed graph on the right.

Finally, the above identification induces a correspondence between elements of $\mathfrak{sDer}_k$ and the graded vector space spanned by internally connected, internally trivalent, internally tree, undirected graphs with k external vertices modulo the IHX relation. The identification goes as follows: For such an undirected graph G and $i \in \{1, \dots, k\}$ we choose an edge $e = (i, v)$ of the external vertex i and orient it away from i. The vertex v then becomes our root and the orientation of all other edges is automatically given by the fact that all internal vertices of G are trivalent, G is an internal tree and that every internal vertex should have one incoming and two outgoing edges. Repeat this procedure for every edge of i and every external vertex $i \in \{1, \dots, k\}$.

The sign of each graph is then fixed by the following convention: The edges of the tree should be ordered such that the edge from (i, v) comes first. Then the two outgoing edges of the root e, e' and afterwards all edges of the subtree whose incoming edge is e and then all edges of the subtree whose incoming edge is e' where w.l.o.g. we assume that $|e| < |e'|$. We call the subtree corresponding to e the left and the one corresponding to e' the right subtree. Apply this convention then recursively on all subtrees. This gives a graph that corresponds to an element of $\mathfrak{tDer}_k$ by the above described identification. In particular it is an element of $\mathfrak{sDer}_k$ and can then be converted into a Lie word. What remains to show is that the ordering fixing the sign is well defined. The following lemma takes care of that:

Lemma 4.21. *The above described construction respects the anti-symmetry relation of the Lie bracket.*

Proof. To show that the construction is well-defined under the anti-symmetry relation means showing that if we exchange the numbering on the two outgoing edges of an internal vertex the sign of the graph flips. This exchange is equivalent to exchanging the two arguments of a Lie Bracket and thus we need this sign change to satisfy the anti-symmetry relation.

By the construction of the ordering on such a graph we know that there exist $j \in \mathbb{N}$ such that the two outgoing edges (v, w_1) and (v, w_2) at a vertex v have order number j and $j + 1$ respectively. We call the subtree corresponding to the edge (v, w_1) the left subtree and the subtree corresponding to the edge (v, w_2) the right subtree. Then from the construction of the ordering we know that there exist $k > j$ and $l > k$ such that the edges in the left subtree of v, have order numbers $j + 2, \dots, k$ and that the edges appearing in the right subtree of v have order numbers $k + 1, \dots, l$.

To then obtain a valid ordering on the graph after exchanging the labels j and $j + 1$ we need to reorder the edges in the subtrees such that all labels in the left subtree are bigger than all labels in the right subtree and the same holds for all further subtrees. This can be achieved by applying the permutation $(j + 2; \dots; k; k + 1; \dots; l)$ a number of $k - (j + 1)$ times. Importantly, every subtree contains an even number of edges and thus $k - (j + 1)$ is even. Therefore, this permutation is even and does not change the sign.

However, the permutation $(j; j + 1)$ remains to exchange the labels on the outgoing edges of v. Hence, the total permutation we need to apply is $(j; j+1)(j+2; \dots; l)^{k-(j+1)}$, which is odd and the sign of the graph flips. This shows the desired result. ☐

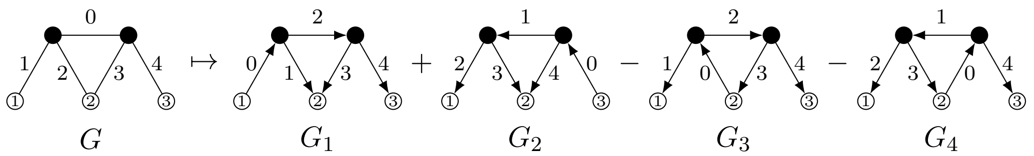


Figure 9: An undirected internally trivalent, internally connected, internally tree graph with 3 external vertices on the left and its image under the correspondence to $\mathfrak{sder}_3$ on the right.

Example 4.22. Consider the graph G as given in Figure 9 on the left. Then in the same image on the right the result of the above identification can be seen. Here The signs come from the application of the permutation $(0;1;2)$ to G_1, $(0;2)$ to G_2, $(4;3;2;1;0)$ to G_3 and $(0;3;2;1)$ to G_4. Moreover, we see that the graph G_1 contributes to u_1, G_2 to u_3 and G_3, G_4 to u_3. We therefore get that the element of $\mathfrak{sder}_3$ corresponding to G is given by

$$u = (u_1, u_2, u_3) = ([Y,[Y,Z]], -[X,[Y,Z]] - [[X,Y],Z], [[X,Y],Y]),$$

where we identified x_1, x_2, x_3 with X, Y, Z. We can now check that this element satisfies the special relation: We have

$$\begin{aligned}[X,u_1] &= [X,[Y,[Y,Z]]] = [[Y,Z],[Y,X]] - [Y,[[Y,Z],X]] \\ [Z,u_3] &= [Z,[Y,[Y,X]]] = [[Y,X],[Y,Z]] - [Y,[[Y,X],Z]] \\ [Y,u_2] &= [Y,[[Y,Z],X]] + [Y,[[Y,X],Z]]\end{aligned}$$

where in the first two lines we used the Jacobi identity and in the last row we just used linearity and anti symmetry. Finally we get

$$[X,u_1] + [Y,u_2] + [Z,u_3] = [[Y,Z],[Y,X]] + [[Y,X],[Y,Z]] = 0$$

by anti-symmetry. Thus, u is an element of $\mathfrak{sder}_3$.

4.5 The map from GC to $\mathfrak{sder}_2$

The goal of this section it to understand Algorithm 1 from [22] which describes the isomorphism between $H^0(\mathsf{GC})$ and $\mathfrak{grt}_1$ in detail. Moreover it will follow that there is a map $\phi : \mathsf{GC} \to \mathfrak{sder}_2$ which when passing to cohomology gives the isomorphism from $H^0(\mathsf{GC})$ to $\mathfrak{grt}_1$. The algorithm is given as follows: Let $\gamma \in \mathsf{GC}$ be a cocycle.

1. We can assume that γ is 1-vertex irreducible.
2. For each graph in γ sum over all ways to mark a vertex as external. This gives a (linear combination of) graph(s) $\gamma_1 \in \mathsf{graphs}(1)$.
3. Split the marked vertex into two and sum over all possible ways to reconnect the incoming edges such that each vertex is hit by at least one edge. Call this linear combination of graphs $\gamma_2' \in \mathsf{ICG}(2)$.
4. γ_2' is closed in $\mathsf{ICG}(2)$ and has no one-edge component, hence it is the coboundary of some element γ_2. We choose γ_2 to be symmetric under interchange of the external vertices 1 and 2.
5. Forget the non-internal-trivalent non-internal-tree part of γ_2 to obtain T.
6. For each tree t occuring in T construct a Lie word in variables X, Y as follows. For each edge incident to vertex 1, cut it and make it the "root" edge. The resulting (internal) tree is a binary tree with leaves labelled by 1 or 2. It can be seen as a Lie tree, and one gets a Lie word $\psi_1(X,Y)$ by replacing each 1 by X and each 2 by Y. Set $\psi(X,Y) =$

$\psi_1(X,Y) - \psi_1(Y,X)$. Summing over all such Lie words one gets a linear combination of Lie words corresponding to γ. Let us call it again $\psi_\gamma(X,Y) \in \mathbb{F}_{\text{Lie}}(X,Y)$.

7. ψ_γ is the desired $\mathfrak{grt}_1$-element.

In the following we are going to describe the steps of this algorithm in detail:

Step 1

This follows from the following proposition:

Proposition 4.23. $\mathsf{GC}_{1vi} \hookrightarrow \mathsf{GC}$ *is a quasi isomorphism.*

Here GC_{1vi} denotes the subspace of 1-vertex irreducible graphs of GC. This result has been shown by Conant, Gerlits and Vogtman in [10].

Steps 2, 3 and 4

Here we follow the extra construction from Rossi and Willwacher from [18, Section 7.3]. Notice that step 3 can explicitly be written down as

$$\gamma_2' = \gamma_1 \circ_1 \Gamma_{\circ\,\circ} - \Gamma_{\circ\,\circ} \circ_1 \gamma_1$$

where $\Gamma_{\circ\,\circ}$ is the graph given by two external vertices and no edges and 1 is the one external vertex. Here the first term corresponds to splitting the external vertex into two and reconnecting the edges in all possible ways. The second term then cancels all the terms of the first where one external vertex is not hit by any edge. We can however also express the steps 2, 3 and 4 via another construction: Consider the map $\psi : \mathsf{GC} \to \mathsf{graphs}(2)$ which works on a Graph G by

$$\psi(G) = \sum_{e=\{u,v\}\in E} (-1)^{|e|-1} \left((G \setminus e)_{u,v} + (G \setminus e)_{v,u}\right),$$

where $G \setminus e$ denotes the graph where e has been deleted from G and $(\ldots)_{u,v}$ denotes the graph where the vertex u has been marked as external with number 1 and v as external with number 2. That is ψ sums over all edges e in γ marks the two vertices connected by e as external and deletes the edge e. The sign arising from $(-1)^{|e|-1}$ is the same as assuming that e has position 1 in the ordering.

We then have the following key lemma from [18, Lemma 7.2]:

Lemma 4.24.

$$d_{\mathsf{graphs}}(\psi(\gamma)) - \psi(d_{\mathsf{GC}}(\gamma)) = \gamma_1 \circ \Gamma_{\circ\,\circ} - \Gamma_{\circ\,\circ} \circ \gamma_1$$

Since γ is closed and if we only keep the internally connected part of $\psi(\gamma)$ we get

$$\gamma_2 = \psi(\gamma)$$

as by the lemma

$$d_{\mathsf{graphs}}(\gamma_2) = \gamma_1 \circ \Gamma_{\circ\,\circ} - \Gamma_{\circ\,\circ} \circ \gamma_1 + \psi(d_{\mathsf{GC}}(\gamma)) = \gamma_2' + 0 = \gamma_2'.$$

This also instantly shows that γ_2' is closed as $d_{\mathsf{graphs}}(\gamma_2') = d^2_{\mathsf{graphs}}(\gamma_2) = 0$ and clearly it is also a coboundary as $d_{\mathsf{graphs}}(\gamma_2) = \gamma_2'$. This last statement however follows also for general elements of $\mathsf{ICG}(2)$:

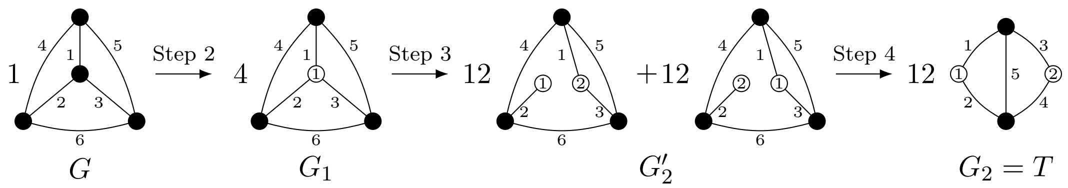
Proposition 4.25. *A closed element of* $\mathsf{ICG}(2)$ *with no one-edge component is a co-boundary.*

Proof. Notice that the only generator of $H^*(\mathsf{ICG}(2))$ is given by the graph corresponding to t_{12} which is exactly $\Gamma_{\circ\!-\!\circ}$, the graph with two external vertices connected by an edge. As the only possible product is $[t_{12}, t_{12}] = 0$ the homology of $\mathsf{ICG}(2)$ is given by $\mathbb{Q} \cdot \Gamma_{\circ\!-\!\circ}$.

Now if a closed element G contains no one-edge component then it cannot contain the generator $\Gamma_{\circ\!-\!\circ}$ and thus must vanish in homology. This implies that there exists H such that $G = d_{\mathsf{graphs}}(H)$ and thus G is a co-boundary. $\square$

To illustrate these three steps we can consider the following example:

Example 4.26. Let G be the three wheel graph. Then G is a co-cycle as no vertex of G can be split into two ≥ 3-valent vertices. The figure below illustrates G, G_1, G_2' and G_2 as well as T from Step 5.



A further example of these computations can be found in Appendix A for the five wheel.

Step 5

This step is rather straightforward and does not warrant any further explanation. However, this step is also very restricting in the graphs that contribute to the final result. This can be seen as follows:

Definition 4.27. As the fundamental group of a graph G is isomorphic to the free group we can define the *rank of a graph* $\text{rank}(G)$ to be the rank of its fundamental group. It can be shown that this is equal to

$$\text{rank}(G) = |E| - |V| + 1,$$

that is the *Euler characteristic of* G.

Notice now that for an element of $H^0(\mathsf{GC})$ it holds that $2\,\text{rank}(G) = |E|$:

$$0 = \deg(G) = 2|V| - E - 2 \Rightarrow -|E| = -(2|E| - 2|V| + 2) = 2\,\text{rank}(G).$$

Consider the map ψ. Then we observe that, for a graph $G_2 = \psi(G)$ to be internally trivalent all but two vertices of G need to be trivalent. Moreover, the two non trivalent vertices needed to be chosen as external. We denote them by v_1, v_2 and their degrees by d_1 and d_2.

Using the handshaking lemma, that is for every undirected graph the following holds

$$\sum_{v \in V} \deg(v) = 2E,$$

and the definition of the rank we find

$$\begin{aligned} 2E = \sum_{v \in V} \deg(v) &= 3 \cdot (V - 2) + d_1 + d_2 = 3(E - \text{rank}(G) - 1) + d_1 + d_2 \\ \Rightarrow d_1 + d_2 &= 3(\text{rank}(G) + 1) - E = \text{rank}(G) + 3 \end{aligned}$$

where in the first line we used the handshaking lemma in the first equality and the fact that $V = E - \text{rank}(G) + 1$ in the third equality. In the second line we used that $E = 2\,\text{rank}(G)$.

Thus, we see that the only contributing graphs are graphs that are trivalent on all but two vertices and whose degree on the final two vertices satisfies $d_1 + d_2 = \text{rank}(G) + 3$.

Step 6

Although step 6 can be executed as given in the algorithm one can also perform it via the identification between $\mathfrak{sder}_k$ and the graded vector space spanned by internally connected, internally trivalent, internally tree, undirected graphs given in Section 4.4.

For this we consider the element $u = (u_1, u_2)$ corresponding to T via this identification. Then we have that $\psi_1(X, Y)$ is equal to u_1 and $\psi_1(Y, X)$ is equal to u_2. This follows as by the requirements in step 4, T is symmetric under interchange of the external vertices and thus making the edges incident to vertex 1 the root edges and naming 1 Y and 2 X is the same as making the edges incident to vertex 2 the root edges and naming 1 X and 2 Y. This is exactly what gives u_2. Therefore, under this identification we have that $\psi_\gamma(X, Y) = u_1 - u_2$.

Using the alternative description of steps 2, 3 and 4 via the map ψ this gives a map $\phi : \mathsf{GC} \to \mathfrak{sder}_2$ by $\phi(G) = \psi_\gamma(X, Y)$.

Example 4.28. Continuing from Example 4.26 by applying this identification we find that the element in $\mathfrak{grt}_1$ corresponding to the three wheel is given by

$$\sigma_3 := -24 \cdot [X, [X, Y]] + 24 \cdot [[X, Y], Y].$$

The result for the five wheel can also be found in Appendix A as well as for the seven wheel in Appendix B.

4.6 Calculating τ_{2j+1} to weight 13

In this section we are going to use the implementation of the map ϕ as well as the formulas derived for $c_{2n}, c_{\alpha,\beta}, c_{\alpha,\beta,\gamma}$ to calculate τ_k for $k \leq 13$ odd.

First however we need the following result about the term $\text{ad}_x^{2n}(y)$ and the wheel graph:

Proposition 4.29. *Let $n \in \mathbb{N}$. The pre-image of $\text{ad}_x^{2n}(y)$ in $\mathfrak{grt}_1$ under the above isomorphism is given by the $2n + 1$ wheel-graph as given in Figure 2. That is under the above isomorphism the only graph that gives the term $\text{ad}_x^{2n}(y)$ is the wheel graph.*

Proof. Assume that $G \in \mathsf{GC}$ such that $\text{ad}_x^{2n}(y) \in \text{Im}(\phi\mid_G)$. Then G has $2n + 2$ vertices as $\phi(G)$ gives words of lengths $2n+1$ exactly if it contains $2n+2$ vertices as two vertices are being chosen as external and then each other vertex gives one bracket. We denote the external vertices by x and y. From step 5 we know that $G \setminus \{x, y\}$ is a tree and thus has $(|V_G|-2)-1$ edges. Moreover, from step 4 we know that there is an edge between x and y in G. Let us denote the degree of x, y be d_x, d_y respectively. From this we conclude that

$$|E_G| = (|V_G| - 2) - 1 + d_x + d_y - 1$$

On the other hand, however, we have that each internal vertex is trivalent and thus by the handshaking lemma we have

$$2|E_G| = 3(|V_G| - 2) + d_x + d_y.$$

By combining the two results we find that $d_x + d_y = |V_G| + 2$. Now trivially we have that $d_x \leq |V_G| - 1$. Furthermore, $d_1 \leq 3$ as else we would get more than one y in the words in $\phi(G)$ (one edge is between x and y, another edge could go to the root and one final edge then gives the one y). This, however, implies that $d_x = |V_G| - 1$ and $d_y = 3$. This means that x is connected to every vertex in G and thus $G \setminus \{x\}$ is bivalent. Moreover, as G needs to be internally connected to contribute and y is connected to at least one internal vertex $G \setminus \{x\}$ is connected. However, the only connected bivalent graph on k vertices is the k-cycle. Thus, $G \setminus \{x\}$ is the k-cycle and G is then the $2n+1$-wheel. This shows the result. □

Let us denote by σ_3, σ_5 and σ_7 the cocycles as defined in Example 4.28, Appendix A and Appendix B respectively. Then notice that the dimension for $\mathfrak{grt}_1$ in degree 3, 5 and 7 is 1 (cf. [15], Table 1). Therefore, if we find the coefficient of $\mathrm{ad}_x^{k-1}(y)$ (or any other Lie word of weight k) for $k \in \{3,5,7\}$ we can infer the complete description of the τ_3, τ_5 and τ_7. Now, by the above Lemma 4.29 we know that only the 3, 5 and 7 wheel contribute to $\mathrm{ad}_x^k(y)$ and thus by calculating the wheels coefficient we get the full description. Doing the calculations we find:

$$\begin{aligned}
\tau_3 &= -\frac{5}{2}\sigma_3 \frac{\zeta(3)}{(2\pi i)^3} = 60\frac{\zeta(3)}{(2\pi i)^3}\left([X,[X,Y]] - [[X,Y],Y]\right) \\
\tau_5 &= 126 \cdot \sigma_5 \frac{\zeta(5)}{(2\pi i)^5} = 630\frac{\zeta(5)}{(2\pi i)^5}(-2\cdot[Y,[Y,[Y,[Y,X]]]] + 4\cdot[Y,[Y,[[Y,X],X]]] \\
&\qquad - 3\cdot[[Y,[Y,X]],[Y,X]] - 4\cdot[Y,[[[Y,X],X],X]] \\
&\qquad - [[Y,X],[[Y,X],X]] + 2\cdot[[[[Y,X],X],X],X]) \\
\tau_7 &= -1716 \cdot \sigma_7 \frac{\zeta(7)}{(2\pi i)^7}.
\end{aligned}$$

For weight 9 we unfortunately do not have a full description of the cocycle. If we define σ_9 up to depth 3 however as

$$\begin{aligned}
\sigma_9 :=\ & \mathrm{ad}_x^8(y) - \frac{i\,\zeta(9)}{128\,\pi^9 e_1}[\mathrm{ad}_x^0(y),\mathrm{ad}_x^7(y)] - \frac{19i\,\zeta(9)}{1024\,\pi^9 e_1}[\mathrm{ad}_x^1(y),\mathrm{ad}_x^6(y)] - \frac{29i\,\zeta(9)}{1024\,\pi^9 e_1}[\mathrm{ad}_x^2(y),\mathrm{ad}_x^5(y)] \\
& - \frac{13i\,\zeta(9)}{1024\,\pi^9 e_1}[\mathrm{ad}_x^3(y),\mathrm{ad}_x^4(y)] + \frac{28}{3}[\mathrm{ad}_x^0(y),[\mathrm{ad}_x^0(y),\mathrm{ad}_x^6(y)]] + \frac{1843}{72}[\mathrm{ad}_x^0(y),[\mathrm{ad}_x^1(y),\mathrm{ad}_x^5(y)]] \\
& + \frac{1217}{72}[\mathrm{ad}_x^1(y),[\mathrm{ad}_x^0(y),\mathrm{ad}_x^5(y)]] + \frac{835}{36}[\mathrm{ad}_x^0(y),[\mathrm{ad}_x^2(y),\mathrm{ad}_x^4(y)]] + \frac{2723}{72}[\mathrm{ad}_x^1(y),[\mathrm{ad}_x^1(y),\mathrm{ad}_x^4(y)]] \\
& + \frac{593}{24}[\mathrm{ad}_x^2(y),[\mathrm{ad}_x^0(y),\mathrm{ad}_x^4(y)]] + \frac{221}{18}[\mathrm{ad}_x^1(y),[\mathrm{ad}_x^2(y),\mathrm{ad}_x^3(y)]] + \frac{1613}{36}[\mathrm{ad}_x^2(y),[\mathrm{ad}_x^1(y),\mathrm{ad}_x^3(y)]] \\
& + \frac{467}{36}[\mathrm{ad}_x^3(y),[\mathrm{ad}_x^0(y),\mathrm{ad}_x^3(y)]] + \dots
\end{aligned}$$

where we normalized such that the coefficient $\mathrm{ad}_x^8(y)$ of the 9 wheel is 1. We have, as the dimension of $\mathfrak{grt}_1$ in weight 9 is still 1, that τ_9 is given by

$$\tau_9 = 437580 \cdot \sigma_9 \frac{\zeta(9)}{(2\pi i)^9}.$$

Finally for weight 11 and 13 we have that the $\mathfrak{grt}_1$ dimensions are 2 and 3. Generators can then be given by $\sigma_{11}, [\sigma_3,[\sigma_3,\sigma_5]_{\mathrm{Ih}}]_{\mathrm{Ih}}$ and $\sigma_{13}, [\sigma_3,[\sigma_3,\sigma_7]_{\mathrm{Ih}}]_{\mathrm{Ih}}, [\sigma_5,[\sigma_5,\sigma_3]_{\mathrm{Ih}}]_{\mathrm{Ih}}$ respectively. Where once again we can only define σ_{11} and σ_{13} up to depth 3 by

$$\begin{aligned}\sigma_{11} = {}& \mathrm{ad}_x^{10}(y) + 5[\mathrm{ad}_x^0(y), \mathrm{ad}_x^9(y)] + 17[\mathrm{ad}_x^1(y), \mathrm{ad}_x^8(y)] + 38[\mathrm{ad}_x^2(y), \mathrm{ad}_x^7(y)] + \frac{89}{2}[\mathrm{ad}_x^3(y), \mathrm{ad}_x^6(y)] \\
&+ \frac{43}{2}[\mathrm{ad}_x^4(y), \mathrm{ad}_x^5(y)] + 15[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^8(y)]] + \frac{7651}{240}[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^7(y)]] \\
&+ \frac{15869}{240}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^7(y)]] - \frac{5063}{240}[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^6(y)]] + \frac{55237}{240}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^6(y)]] \\
&+ \frac{571}{4}[\mathrm{ad}_x^2(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^6(y)]] - \frac{3077}{48}[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^3(y), \mathrm{ad}_x^5(y)]] + \frac{11717}{40}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^5(y)]] \\
&+ \frac{40077}{80}[\mathrm{ad}_x^2(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^5(y)]] + \frac{1757}{30}[\mathrm{ad}_x^3(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^5(y)]] + \frac{8519}{48}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^3(y), \mathrm{ad}_x^4(y)]] \\
&+ \frac{9881}{16}[\mathrm{ad}_x^2(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^4(y)]] + \frac{5581}{48}[\mathrm{ad}_x^3(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^4(y)]] - \frac{417}{16}[\mathrm{ad}_x^4(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^4(y)]] \\
&+ \frac{2701}{24}[\mathrm{ad}_x^3(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^3(y)]] + \ldots\end{aligned}$$

and

$$\begin{aligned}\sigma_{13} = {}& \mathrm{ad}_x^{12}(y) + 6[\mathrm{ad}_x^0(y), \mathrm{ad}_x^{11}(y)] + \frac{53}{2}[\mathrm{ad}_x^1(y), \mathrm{ad}_x^{10}(y)] + \frac{155}{2}[\mathrm{ad}_x^2(y), \mathrm{ad}_x^9(y)] \\
&+ 137[\mathrm{ad}_x^3(y), \mathrm{ad}_x^8(y)] + 149[\mathrm{ad}_x^4(y), \mathrm{ad}_x^7(y)] + \frac{131}{2}[\mathrm{ad}_x^5(y), \mathrm{ad}_x^6(y)] \\
&+ 22[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^{10}(y)]] + \frac{174721}{2100}[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^9(y)]] \\
&+ \frac{219029}{2100}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^9(y)]] + \frac{33619}{350}[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^8(y)]] \\
&+ \frac{328863}{700}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^8(y)]] + \frac{1063}{4}[\mathrm{ad}_x^2(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^8(y)]] \\
&- \frac{4121}{150}[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^3(y), \mathrm{ad}_x^7(y)]] + \frac{144101}{175}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^7(y)]] \\
&+ \frac{210388}{175}[\mathrm{ad}_x^2(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^7(y)]] + \frac{12503}{42}[\mathrm{ad}_x^3(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^7(y)]] \\
&- \frac{20999}{150}[\mathrm{ad}_x^0(y), [\mathrm{ad}_x^4(y), \mathrm{ad}_x^6(y)]] + \frac{49439}{75}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^3(y), \mathrm{ad}_x^6(y)]] \\
&+ \frac{107601}{50}[\mathrm{ad}_x^2(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^6(y)]] + \frac{31546}{25}[\mathrm{ad}_x^3(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^6(y)]] \\
&+ 230[\mathrm{ad}_x^4(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^6(y)]] - \frac{1524}{25}[\mathrm{ad}_x^1(y), [\mathrm{ad}_x^4(y), \mathrm{ad}_x^5(y)]] \\
&+ \frac{38889}{25}[\mathrm{ad}_x^2(y), [\mathrm{ad}_x^3(y), \mathrm{ad}_x^5(y)]] + \frac{52426}{25}[\mathrm{ad}_x^3(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^5(y)]] \\
&+ \frac{27394}{25}[\mathrm{ad}_x^4(y), [\mathrm{ad}_x^1(y), \mathrm{ad}_x^5(y)]] + \frac{5263}{50}[\mathrm{ad}_x^5(y), [\mathrm{ad}_x^0(y), \mathrm{ad}_x^5(y)]] \\
&+ \frac{29023}{30}[\mathrm{ad}_x^3(y), [\mathrm{ad}_x^3(y), \mathrm{ad}_x^4(y)]] + \frac{9949}{10}[\mathrm{ad}_x^4(y), [\mathrm{ad}_x^2(y), \mathrm{ad}_x^4(y)]] + \ldots.\end{aligned}$$

where we also normalized such that the coefficient of $\mathrm{ad}_x^{10}(y)$ and $\mathrm{ad}_x^{12}(y)$ of the 11 and 13 wheel are 1 respectively. With this defined we find for τ_{11} and τ_{13} :

$$\tau_{11} = 7759752 \cdot \sigma_{11}\frac{\zeta(11)}{(2\pi i)^{11}} + \left(-\frac{323323}{2400} \cdot [\sigma_3, [\sigma_3, \sigma_5]_{\mathrm{Ih}}]_{\mathrm{Ih}}\right)\left(\frac{\zeta_{\mathrm{sv}}(5,3,3)}{(2\pi i)^{11}} + \frac{22020}{3553}\frac{\zeta(3)^2\zeta(5)}{(2\pi i)^{11}}\right)$$

and

$$\tau_{13} = \frac{\zeta(13)}{(2\pi i)^{13}} \cdot (135207800 \cdot \sigma_{13})$$
$$+ \left(\frac{2414425}{4032} \cdot [\sigma_3, [\sigma_3, \sigma_7]_{\mathrm{Ih}}]_{\mathrm{Ih}}\right) \left(\frac{\zeta_{\mathrm{sv}}(7,3,3)}{(2\pi i)^{13}} - \frac{244740}{5681}\frac{\zeta(5)^2\zeta(3)}{(2\pi i)^{13}} + \frac{123508}{7429}\frac{\zeta(7)\zeta(3)^2}{(2\pi i)^{13}}\right)$$
$$+ \left(-\frac{676039}{600} \cdot [\sigma_5, [\sigma_5, \sigma_3]_{\mathrm{Ih}}]_{\mathrm{Ih}} - \frac{482885}{672} \cdot [\sigma_3, [\sigma_3, \sigma_7]_{\mathrm{Ih}}]_{\mathrm{Ih}}\right) \left(\frac{\zeta_{\mathrm{sv}}(5,5,3)}{(2\pi i)^{13}} - \frac{203950}{5681}\frac{\zeta(5)^2\zeta(3)}{(2\pi i)^{13}}\right).$$

Notice importantly that even though we only know the values up to depth 3 we get far more information from this. In particular, in principle in weight 9 the MZV $\zeta(5,3)$ could appear however in the coefficients up to depth 3 it does not and thus by the dimension constraint it can also not appear in higher depths. Similarly, for τ_{11} and τ_{13} for all MZVs but $\zeta(11)$ and $\zeta(13)$ we know the total contribution of all depths even though once again we only calculated the coefficients up to depth 3. In this case this works by the dimension constraint and the fact that we know the full description of the generators $[\sigma_3, [\sigma_3, \sigma_5]_{\mathrm{Ih}}]_{\mathrm{Ih}}$ and $[\sigma_3, [\sigma_3, \sigma_7]_{\mathrm{Ih}}]_{\mathrm{Ih}}, [\sigma_5, [\sigma_5, \sigma_3]_{\mathrm{Ih}}]_{\mathrm{Ih}}$ respectively.

For higher weights, i.e. ≥ 15, quadruple MZVs appear in the conjectured basis of MZVs. As these appear only for depths ≥ 4 we cannot obtain them here and thus weight 13 is the maximum where a reasonable description of τ_k can be given with calculations only up to depth 3.

5 Remaining proofs

Proof of Lemma 3.10. Let $a, b, c, d \in \mathbb{N}_0$ and let $N := a + b + c + d$. Moreover, let $w = x^a y x^b y x^x y x^d$. Let us first consider the terms given by the action of $I_t^s c_{\alpha,\beta}\left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right]$ on elements of degree 1. This is given by:

$$I_t^s c_{\alpha,\beta}\left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right] \cdot (x^p y x^q) + \left[y, I_t^s c_{\alpha,\beta}\left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right]\right] \cdot \partial_y(x^p y x^q), \tag{8}$$

where $s \in \mathbb{N}$, $p, q \in \mathbb{N}_0$ such that $\alpha + \beta = 2s - 1$ and $2s - 1 + p + q = N$. Expanding the first term yields

$$I_t^s c_{\alpha,\beta} \sum_{i=0}^{\alpha}\sum_{j=0}^{\beta} \binom{\alpha}{i}\binom{\beta}{j}(-1)^{i+j}\left(x^i y x^{\alpha-i+j} y x^{\beta-j+p} y x^q - x^j y x^{\beta-j+i} y x^{\alpha-i+p} y x^q\right)$$

This contributes with the first term when $q = d$, $i = a$, $j = b + a - \alpha$ and $p = b + a + c - (2s - 1)$ and with the second if $q = d$, $j = a$, $i = b + a - \beta$ and $p = b + a + c - (2s - 1)$. Therefore, the terms we are interested in are given by

$$\sum_{\substack{s\in\mathbb{N}, p\in\mathbb{N}_0\\ \alpha+\beta=2s-1\\ p=a+b+c-(2s-1)}} I_t^s c_{\alpha,\beta}\left(\binom{\alpha}{a}\binom{\beta}{b+a-\alpha}(-1)^{b-\alpha} - \binom{\alpha}{b+a-\beta}\binom{\beta}{a}(-1)^{b-\beta}\right) u_{x^p y x^d}.$$

Expanding the second term in equation (8) gives:

$$I_t^s c_{\alpha,\beta} x^p \left[y, \left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right]\right] x^q = I_t^s c_{\alpha,\beta} \sum_{i=0}^{\alpha}\sum_{j=0}^{\beta}\binom{\alpha}{i}\binom{\beta}{j}(-1)^{i+j}(x^p y x^i y x^{\alpha-i+j} y x^{\beta-j+q}$$
$$- x^{p+i} y x^{\alpha-i+j} y x^{\beta-j} y x^q - x^p y x^j y x^{\beta-j+i} y x^{\alpha-i+q} + x^{p+j} y x^{\beta-j+i} y x^{\alpha-i} y x^q).$$

This contributes with

- the first term if $p = a$, $i = b$, $j = b + c - \alpha$ and $q = b + c + d - (2s - 1)$,
- the second term if $q = d$, $j = \beta - c$, $i = \alpha + \beta - b - c$ and $p = a + b + c - (2s - 1)$,
- the third term if $p = a$, $j = b$, $i = b + c - \beta$ and $q = b + c + d - (2s - 1)$,
- the fourth term if $q = d$, $i = \alpha - c$, $j = \alpha + \beta - b - c$ and $p = a + b + c - (2s - 1)$.

The terms we are interested in are thus given by

$$\sum_{\substack{s\in\mathbb{N},p\in\mathbb{N}_0\\ \alpha+\beta=2s-1\\ p=a+b+c-(2s-1)}} I_t^s c_{\alpha,\beta}\left(\binom{\alpha}{b+c-\beta}\binom{\beta}{c}(-1)^{b-\beta} - \binom{\alpha}{c}\binom{\beta}{b+c-\alpha}(-1)^{b-\alpha}\right)u_{x^pyx^d}$$
$$+\sum_{\substack{s\in\mathbb{N},p\in\mathbb{N}_0\\ \alpha+\beta=2s-1\\ p=b+c+d-(2s-1)}} I_t^s c_{\alpha,\beta}\left(\binom{\alpha}{b}\binom{\beta}{b+c-\alpha}(-1)^{c-\alpha} - \binom{\alpha}{b+c-\beta}\binom{\beta}{b}(-1)^{c-\beta}\right)u_{x^pyx^d}.$$

Secondly, we get the action of $I_t^s c_{2s}\operatorname{ad}_x^{2s}(y)$ on elements of degree 2. This gives:

$$I_t^s c_{2s}\operatorname{ad}_x^{2s}(y)(x^pyx^qyx^r) + \left[y, I_t^s c_{2s}\operatorname{ad}_x^{2s}(y)\right]\partial_y(x^pyx^qyx^r) \tag{9}$$

where $s \in \mathbb{N}, p, q, r \in \mathbb{N}_0$ such that $2s + p + q + r = N$. Expanding the first term yields

$$I_t^s c_{2s}\sum_{i=0}^{2s}\binom{2s}{i}(-1)^i x^i y x^{2s-i+p} y x^q y x^r.$$

This contributes if $i = a$, $q = c$, $r = d$ and $p = a + b - 2s$. Thus, the terms we are interested in are given by

$$\sum_{\substack{s\in\mathbb{N},p\in\mathbb{N}_0\\ p=a+b-2s}} I_t^s c_{2s}(-1)^a\binom{2s}{a}u_{x^pyx^cyx^d}.$$

Considering the second term in equation (9) gives

$$\left[y, I_t^s c_{2s}\operatorname{ad}_x^{2s}(y)\right]\partial_y(x^pyx^qyx^r) = I_t^s c_{2s}\sum_{i=0}^{2s}\binom{2s}{i}(-1)^i(x^pyx^iyx^{2s-i+q}yx^r$$
$$- x^{p+i}yx^{2s-i}yx^qyx^r + x^pyx^qyx^iyx^{2s-i+r} - x^pyx^{q+i}yx^qyx^r).$$

This contributes with

- the first term when $p = a$, $i = b$, $r = d$ and $q = b + c - 2s$,
- the second term when $q = c$, $r = d$, $i = 2s - b$ and $p = a + b - 2s$,
- the third term when $p = a$, $q = b$, $i = c$ and $r = d + c - 2s$,
- the fourth term when $p = a$, $r = d$, $i = 2s - c$ and $q = b + c - 2s$.

The terms we are interested in are thus given by

$$+\sum_{2s=b+c-q} I_1^{2s}c_{2s}\left(\binom{2s}{b}(-1)^b - \binom{2s}{c}(-1)^c\right)u_{x^ayx^qyx^d}$$
$$-\sum_{2s=a+b-p} I_1^{2s}c_{2s}\binom{2s}{b}(-1)^b u_{x^pyx^cyx^d} + \sum_{2s=c+d-r} I_1^{2s}c_{2s}\binom{2s}{c}(-1)^c u_{x^ayx^byx^r}.$$

This shows the desired result. □

Proof of Lemma 3.11. Let us first expand the following expression

$$\mathrm{ad}_x^l(y) \circ (\mathrm{ad}_x^m(y) \circ x^p y x^q)$$

with $\circ$ being the action from Definition 2.25 and $l, m \in \mathbb{N}$ and $p, q \in \mathbb{N}_0$. In the following we call the terms ab the first part of the action $a \circ b$ and the terms $[y, a]\partial_y b$ the second part of the action. Expanding the term in brackets gives:

$$\sum_{j=0}^{2m} \binom{2m}{j} \left(x^j y x^{2m-j+p} y x^q + x^p y x^j y x^{2m-j+q} - x^{p+j} y x^{2m-j} y x^q \right).$$

Let us now consider the first part of the action of $\mathrm{ad}_x^l(y)$ on this expression. This gives:

$$\sum_{i=0}^{2l} \sum_{j=0}^{2m} \binom{2l}{i} \binom{2m}{j} (-1)^{i+j} \Big(x^i y x^{2l-i+j} y x^{2m-j+p} y x^q + x^i y x^{2l-i+p} y x^j y x^{2m-j+q} \\ - x^i y x^{2l-i+p+j} y x^{2m-j} y x^q \Big).$$

If we only consider the terms that contain w we get that this contributes with

- the first term if $i = a$, $j = a + b - 2l$, $p = a + b + c - 2l - 2m$ and $q = d$,
- the second term if $i = a$, $j = c$, $p = a + b - 2l$ and $q = c + d - 2m$,
- the third term if $i = a$, $j = 2m - c$, $p = a + b + c - 2l - 2m$ and $q = d$.

Considering the second part of the action we get:

$$\sum_{i=0}^{2l} \sum_{j=0}^{2m} \binom{2l}{i} \binom{2m}{j} (-1)^{i+j} \Big(x^j y x^i y x^{2l+2m-i-j+p} y x^q - x^{i+j} y x^{2l-i} y x^{2m-j+p} y x^q \\ + x^j y x^{2m-j+p} y x^i y x^{2l-i+q} - x^j y x^{2m-j+p+i} y x^{2l-i} y x^q + x^p y x^i y x^{2l-i+j} y x^{2m-j+q} \\ - x^{p+i} y x^{2l-i} y x^j y x^{2m-j+q} + x^p y x^j y x^i y x^{2l+2m-i-j+q} - x^p y x^{i+j} y x^{2l-i} y x^{2m-j+q} \\ - x^{p+j} y x^i y x^{2l+2m-i-j} y x^q + x^{p+j+i} y x^{2l-i} y x^{2m-j} y x^q - x^{p+j} y x^{2m-j} y x^i y x^{2l-i+q} \\ + x^{p+j} y x^{2m-j+i} y x^{2l-i} y x^q \Big).$$

This contributes with

- the 1st term if $i = b$, $j = a$, $p = a + b + c - 2l - 2m$ and $q = d$,
- the 2nd term if $i = 2l - b$, $j = a + b - 2l$, $p = q + b + c - 2l - 2m$ and $q = d$,
- the 3rd term if $i = c$, $j = a$, $p = a + b - 2m$ and $q = c + d - 2l$,
- the 4th term if $i = 2l - c$, $j = a$, $p = a + b + c - 2l - 2m$ and $q = d$,
- the 5th term if $i = b$, $j = b + c - 2l$, $p = a$ and $q = b + c + d - 2l - 2m$,
- the 6th term if $i = 2l - b$, $j = c$, $p = a + b - 2l$ and $q = c + d - 2m$,
- the 7th term if $i = c$, $j = b$, $p = a$ and $q = b + c + d - 2l - 2m$,
- the 8th term if $i = 2l - c$, $j = b + c - 2l$, $p = a$ and $q = b + c + d - 2l - 2m$,
- the 9th term if $i = b$, $j = 2m - (b + c - 2l)$, $p = a + b + c - 2l - 2m$ and $q = d$,
- the 10th term if $i = 2l - b$, $j = 2m - c$, $p = a + b + c - 2l - 2m$ and $q = d$,
- the 11th term if $i = c$, $j = 2m - b$, $p = a + b - 2m$ and $q = c + d - 2l$,
- the 12th term if $i = 2l - c$, $j = 2m - (b + c - 2l)$, $p = a + b + c - 2l - 2m$ and $q = d$.

In the case of the double integrals the factor $J_t^{l,m} c_{2l} c_{2m}$ coming from the ψ part and the factor $u_{x^p y x^q}$ from the Φ_{KZ} contribute extra to everyone of these terms. Collecting all the terms then gives

$$\sum_{\substack{l,m\in\mathbb{N},p\in\mathbb{N}_0\\p=a+b+c-2l-2m}} J_t^{l,m}c_{2l}c_{2m}\left(\binom{2l}{a}\binom{2m}{a+b-2l}(-1)^b-\binom{2l}{a}\binom{2m}{c}(-1)^{a-c}+\binom{2l}{b}\binom{2m}{a}(-1)^{a+b}\right.$$
$$-\binom{2l}{b}\binom{2m}{a+b-2l}(-1)^a-\binom{2l}{c}\binom{2m}{a}(-1)^{a-c}-\binom{2l}{b}\binom{2m}{b+c-2l}(-1)^c$$
$$\left.+\binom{2l}{b}\binom{2m}{c}(-1)^{b+c}+\binom{2l}{c}\binom{2m}{b+c-2l}(-1)^b\right)u_{x^pyx^d}$$
$$+\sum_{\substack{l,m\in\mathbb{N},q\in\mathbb{N}_0\\q=b+c+d-2l-2m}} J_t^{l,m}c_{2l}c_{2m}\left(\binom{2l}{b}\binom{2m}{b+c-2l}(-1)^c\right.$$
$$\left.+\binom{2l}{c}\binom{2m}{b}(-1)^{b+c}-\binom{2l}{c}\binom{2m}{b+c-2l}(-1)^b\right)u_{x^ayx^q}$$
$$+\sum_{\substack{l,m\in\mathbb{N},p,q\in\mathbb{N}_0\\p=a+b-2m\\q=c+d-2l}} J_t^{l,m}c_{2l}c_{2m}\left(\binom{2l}{c}\binom{2m}{a}(-1)^{a+c}-\binom{2l}{c}\binom{2m}{b}(-1)^{c-b}\right)u_{x^pyx^q}$$
$$+\sum_{\substack{l,m\in\mathbb{N},p,q\in\mathbb{N}_0\\p=a+b-2l\\q=c+d-2m}} J_t^{l,m}c_{2l}c_{2m}\left(\binom{2l}{a}\binom{2m}{c}(-1)^{a+c}-\binom{2l}{b}\binom{2m}{c}(-1)^{c-b}\right)u_{x^pyx^q}.$$

Finally notice that by relabelling l, m in the last sum to m, l we obtain that the last sum is the same as the second to last which gives the desired result. ☐

Proof of Lemma 3.12. Let us first consider the expression

$$\left[\mathrm{ad}_x^\alpha(y), \mathrm{ad}_x^\beta(y)\right]\circ\left(\mathrm{ad}_x^{2m}(y)\circ 1\right)$$

with $\circ$ being the action from Definition 2.25, $\alpha+\beta=2l-1$ and $l, m\in\mathbb{N}$. In the following we call the terms ab the first part of the action $a\circ b$ and the terms $[y,a]\partial_y b$ the second part of the action. The first part of the action gives:

$$\sum_{i,j,k}\binom{\alpha}{i}\binom{\beta}{j}\binom{2m}{k}(-1)^{i+j+k}\left(x^iyx^{\alpha-i+j}yx^{\beta-j+k}yx^{2l-k}-x^jyx^{\beta-j+i}yx^{\alpha-i+k}yx^{2l-k}\right).$$

Only considering the terms that contain w we get that this contributes with

- the first term if $i=a$, $j=a+b-\alpha$ and $k=2m-d$,
- the second term if $i=a+b-\beta$, $j=a$ and $k=2m-d$.

Considering the second part of the action we get

$$\sum_{i,j,k}\binom{\alpha}{i}\binom{\beta}{j}\binom{2m}{k}(-1)^{i+j+k}\left(x^kyx^iyx^{\alpha-i+j}yx^{\beta-j+2m-k}-x^{k+i}yx^{\alpha-i+j}yx^{\beta-j}yx^{2l-k}\right.$$
$$\left.-x^kyx^jyx^{\beta-j+i}yx^{\alpha-i+2m-k}+x^{k+j}yx^{\beta-j+i}yx^{\alpha-i}yx^{2m-k}\right).$$

This contributes with

- the 1st term if $i=b$, $j=b+c-\alpha$ and $k=a$,
- the 2nd term if $i=a+d-2m$, $j=\beta-c$ and $k=2m-d$,
- the 3rd term if $i=b+c-\beta$, $j=b$ and $k=a$,

- the 4th term if $i=\alpha-c$, $j=a+d-2m$ and $k=2m-d$.

In the case of the double integrals the factor $J_t^{l,m}c_{\alpha,\beta}c_{2m}$ coming from the ψ part contribute extra to everyone of these terms. Collecting all the terms gives

$$\sum_{\substack{2l+2m=2n-3\\ \alpha+\beta=2l}} J_t^{l,m}c_{\alpha,\beta}c_{2m}\Bigg(\binom{\alpha}{a}\binom{\beta}{a+b-\alpha}\binom{2m}{d}(-1)^{b+d-\alpha}-\binom{\alpha}{a+b-\beta}\binom{\beta}{a}\binom{2m}{d}(-1)^{b+d-\beta}$$
$$+\binom{\alpha}{b}\binom{\beta}{b+c-\alpha}\binom{2m}{a}(-1)^{a+c-\alpha}-\binom{\alpha}{a+d-2m}\binom{\beta}{c}\binom{2m}{d}(-1)^{a+c-\beta}$$
$$-\binom{\alpha}{b+c-\beta}\binom{\beta}{b}\binom{2m}{a}(-1)^{a+c-\beta}+\binom{\alpha}{c}\binom{\beta}{a+d-2m}i\binom{2m}{d}(-1)^{a+c-\alpha}\Bigg)$$

which is the first half of the desired result.

Let us now consider the second term that is the expression

$$\mathrm{ad}_x^{2l}\circ\Big(\Big[\mathrm{ad}_x^{\alpha}(y),\mathrm{ad}_x^{\beta}(y)\Big]\circ 1\Big)$$

with $\circ$ being the action from Definition 2.25 and $l,m,h\in\mathbb{N}$. The first part of the action gives:

$$\sum_{i,j,k}\binom{\alpha}{i}\binom{\beta}{j}\binom{2l}{k}(-1)^{i+j+k}\Big(x^kyx^{2l-k+i}yx^{\alpha-i+j}yx^{\beta-j}-x^kyx^{2l-k+j}yx^{\beta-j+i}yx^{\alpha-i}\Big).$$

Only considering the terms that contain w we get that this contributes with

- the first term if $i=a+b-2l$, $j=\beta-d$ and $k=a$,
- the second term if $i=\alpha-d$, $j=a+b-2l$ and $k=a$.

Considering the second part of the action we get

$$\sum_{i,j,k}\binom{\alpha}{i}\binom{\beta}{j}\binom{2l}{k}\Big(x^iyx^kyx^{2l+\alpha-i+j-k}yx^{\beta-j}-x^{i+k}yx^{2l-k}yx^{\alpha-i+j}yx^{\beta-j}$$
$$+x^iyx^{\alpha-i+j}yx^kyx^{2l+\beta-j-k}-x^iyx^{\alpha-i+j+k}yx^{2l-k}yx^{\beta-j}-x^jyx^kyx^{2l+\beta+i-j-k}yx^{\alpha-i}$$
$$+x^{j+k}yx^{2l-k}yx^{\beta-j+i}yx^{\alpha-i}-x^jyx^{\beta+i-j}yx^kyx^{2l+\alpha-i-k}+x^jyx^{\beta+i-j+k}yx^{2l-k}yx^{\alpha-i}\Big).$$

This contributes with

- the 1st term if $i=a$, $j=\beta-d$ and $k=b$,
- the 2nd term if $i=a+b-2l$, $j=\beta-d$ and $k=2l-b$,
- the 3rd term if $i=a$, $j=a+b-\alpha$ and $k=c$,
- the 4th term if $i=a$, $j=\beta-d$ and $k=2l-c$,
- the 5th term if $i=\alpha-d$, $j=a$ and $k=b$,
- the 6th term if $i=\alpha-d$, $j=a+b-2l$ and $k=2l-b$,
- the 7th term if $i=a+b-\beta$, $j=a$ and $k=c$,
- the 8th term if $i=\alpha-d$, $j=a$ and $k=2l-c$.

In the case of the double integrals the factor $J_t^{l,m}c_{2l}c_{\alpha,\beta}$ coming from the ψ part contribute extra to everyone of these terms. Collecting all the terms gives

$$\sum_{\substack{2l+2m=2n-3\\ \alpha+\beta=2m}} J_t^{l,m} c_{2l} c_{\alpha,\beta} \Bigg(\Bigg(\binom{\alpha}{a+b-2l}\binom{\beta}{d}\binom{2l}{a}(-1)^{b+d-,\beta} - \binom{\alpha}{d}\binom{\beta}{a+b-2l}\binom{2l}{a}(-1)^{b+d-\alpha}$$

$$\binom{\alpha}{a}\binom{\beta}{d}\binom{2l}{b}(-1)^{a+b+d-\beta} - \binom{\alpha}{a+b-2l}\binom{\beta}{d}\binom{2l}{b}(-1)^{a+d-\beta}$$

$$+\binom{\alpha}{a}\binom{\beta}{a+b-\alpha}\binom{2l}{c}(-1)^{b+c-\alpha} - \binom{\alpha}{a}\binom{\beta}{d}\binom{2l}{c}(-1)^{a+c+d-\beta}$$

$$-\binom{\alpha}{d}\binom{\beta}{a}\binom{2l}{b}(-1)^{a+b+d-\alpha} + \binom{\alpha}{d}\binom{\beta}{a+b-2l}\binom{2l}{b}(-1)^{a+d-\alpha}$$

$$-\binom{\alpha}{a+b-\beta}\binom{\beta}{a}\binom{2l}{c}(-1)^{b+c-\beta} + \binom{\alpha}{d}\binom{\beta}{a}\binom{2l}{c}(-1)^{a+c+d-\alpha}\Bigg).$$

Both results together then show the lemma. □

Proof of Lemma 3.13. Let us first expand the following expression

$$\mathrm{ad}_x^l(y) \circ \left(\mathrm{ad}_x^m(y) \circ \mathrm{ad}_x^h(y)\right)$$

with $\circ$ being the action from Definition 2.25 and $l, m, h \in \mathbb{N}$. In the following we call the terms ab the first part of the action $a \circ b$ and the terms $[y, a]\partial_y b$ the second part of the action. Expanding the term in brackets gives

$$\sum_{j=1}^{2m}\sum_{k=1}^{2h}\binom{2m}{j}\binom{2h}{k}(-1)^{j+k}\left(x^j yx^{2m-j+k} yx^{2h-k} + x^k yx^j yx^{2h+2m-j-k} - x^{k+j} yx^{2m-j} yx^{2h-k}\right).$$

Let us now consider the first part of the action of $\mathrm{ad}_x^l(y)$ on this expression. This gives

$$\sum_{i=1}^{2l}\sum_{j=1}^{2m}\sum_{k=1}^{2h}\binom{2l}{i}\binom{2m}{j}\binom{2h}{k}(-1)^{i+j+k}\Big(x^i yx^{2l-i+j} yx^{2m-j+k} yx^{2h-k}$$

$$+x^i yx^{2l-i+k} yx^j yx^{2h+2m-j-k} - x^i yx^{2l-i+j+k} yx^{2m-j} yx^{2h-k}\Big).$$

If we now only consider the terms that contain w we get that this contributes with

- the first term if $i = a$, $j = a + b - 2l$ and $k = 2h - d$,
- the second term if $i = a$, $j = c$ and $k = a + b - 2l$,
- the third term if $i = a$, $j = 2m - c$ and $k = 2h - d$.

Considering the second part of the action we get:

$$\sum_{i=1}^{2l}\sum_{j=1}^{2m}\sum_{k=1}^{2h}\binom{2l}{i}\binom{2m}{j}\binom{2h}{k}(-1)^{i+j+k}\Big(x^j yx^i yx^{2m+2l-j-i+k} yx^{2h-k}$$

$$- x^{i+j} yx^{2l-i} yx^{2m-j+k} yx^{2h-k} + x^j yx^{2m-j+k} yx^i yx^{2l+2h-i-k} - x^j yx^{2m-j+k+i} yx^{2l-i} yx^{2h-k}$$

$$+ x^k yx^i yx^{2l-i+j} yx^{2h+2m-j-k} - x^{k+i} yx^{2l-i} yx^j yx^{2h+2m-j-k} + x^k yx^j yx^i yx^{2h+2m+2l-i-j-k}$$

$$- x^k yx^{i+j} yx^{2l-i} yx^{2h+2m-j-k} - x^{k+j} yx^i yx^{2l+2m-i-j} yx^{2h-k} + x^{k+j+i} yx^{2l-i} yx^{2m-j} yx^{2h-k}$$

$$-x^{k+j} yx^{2m-j} yx^i yx^{2l+2h-i-k} + x^{k+j} yx^{2m-j+i} yx^{2l-i} yx^{2h-k}\Big).$$

This contributes with:

- the 1st term if $i = b$, $j = a$ and $k = 2h - d$,

- the 2nd term if $i = 2l - b$, $j = a + b - 2l$ and $k = 2h - d$,
- the 3rd term if $i = c$, $j = a$ and $k = a + b.2m$,
- the 4th term if $i = 2l - c$, $j = a$ and $k = 2h - d$,
- the 5th term if $i = b$, $j = b + c - 2l$ and $k = a$,
- the 6th term if $i = 2l - b$, $j = c$ and $k = a + b - 2l$,
- the 7th term if $i = c$, $j = b$ and $k = a$,
- the 8th term if $i = 2l - c$, $j = b + c - 2l$ and $k = a$,
- the 9th term if $i = b$, $j = a + d - 2h$ and $k = 2h - d$,
- the 10th term if $i = 2l - b$, $j = 2m - c$ and $k = 2h - d$,
- the 11th term if $i = c$, $j = 2m - b$ and $k = a + b - 2m$,
- the 12th term if $i = 2l - c$, $k = 2h - d$ and $j = a + d - 2h$.

In the case of the triple integrals the factor $K_t^{l,m,h} c_{2l} c_{2m} c_{2h}$ coming from the ψ part contribute extra to everyone of these terms. Collecting all the terms then gives

$$\sum_{l+m+h=n-1} K_t^{l,m,h} c_{2l} c_{2m} c_{2h} \Bigg(\binom{2l}{a}\binom{2m}{a+b-2l}\binom{2h}{d}(-1)^{b-d} + \binom{2l}{a}\binom{2m}{c}\binom{2h}{a+b-2l}(-1)^{b+c}$$
$$- \binom{2l}{a}\binom{2m}{c}\binom{2h}{d}(-1)^{a-c-d} + \binom{2l}{b}\binom{2m}{a}\binom{2h}{d}(-1)^{a+b-d}$$
$$- \binom{2l}{b}\binom{2m}{a+b-2l}\binom{2h}{d}(-1)^{a-d} + \binom{2l}{c}\binom{2m}{a}\binom{2h}{a+b-2m}(-1)^{b+c}$$
$$- \binom{2l}{c}\binom{2m}{a}\binom{2h}{d}(-1)^{a-c-d} + \binom{2l}{b}\binom{2m}{b+c-2l}\binom{2h}{a}(-1)^{a+c}$$
$$- \binom{2l}{b}\binom{2m}{c}\binom{2h}{a+b-2l}(-1)^{a+c} + \binom{2l}{c}\binom{2m}{b}\binom{2h}{a}(-1)^{a+b+c}$$
$$- \binom{2l}{c}\binom{2m}{b+c-2l}\binom{2h}{a}(-1)^{a+b} - \binom{2l}{b}\binom{2m}{a+d-2h}\binom{2h}{d}(-1)^{a+b}$$
$$+ \binom{2l}{b}\binom{2m}{c}\binom{2h}{d}(-1)^{b+c+d} - \binom{2l}{c}\binom{2m}{b}\binom{2h}{a+b-2m}(-1)^{a+c}$$
$$+ \binom{2l}{c}\binom{2m}{a+d-2h}\binom{2h}{d}(-1)^{a-c} \Bigg)$$

which shows the lemma. □

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A The five wheel under the map ϕ

Notice first that the five wheel (see Figure 10 on the left) is not a closed element in GC. For this we need to add the graph G_2 (see Figure 10 on the right). It can then easily be checked that then $G_1 - \frac{5}{2}G_2$ is closed we call this element γ.

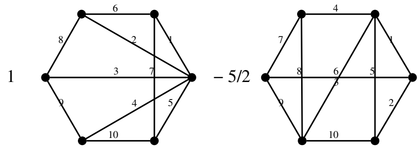

Figure 10: The five wheel G_1 on the left and the auxiliary graph G_2 on the right

In Figure 11 the element γ_1 from step 2 can be seen. In Figure 13 the element γ_2' from step 3 is shown. Moreover, in Figure 12 the element γ_2 obtained via the map ψ is displayed. In Figure 14 the element T obtained in step 5 is depicted. In Figure 15 the directed graphs depicting the element in $\mathfrak{tder}_2$ are shown. Finally the element σ_5 in $\mathfrak{grt}_1$ is given by

$$\begin{aligned}\sigma_5 :=& -10 \cdot [Y,[Y,[Y,[Y,X]]]] + 20 \cdot [Y,[Y,[[Y,X],X]]] - 15 \cdot [[Y,[Y,X]],[Y,X]] \\ & - 20 \cdot [Y,[[[Y,X],X],X]] - 5 \cdot [[Y,X],[[Y,X],X]] + 10 \cdot [[[[Y,X],X],X],X].\end{aligned}$$

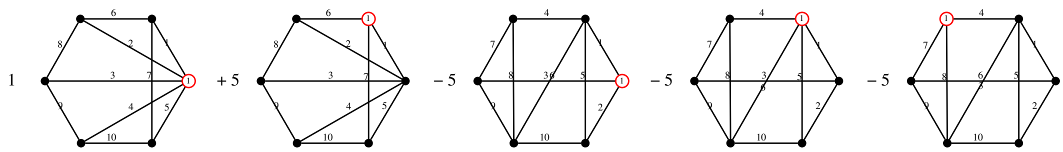

Figure 11: The element γ_1

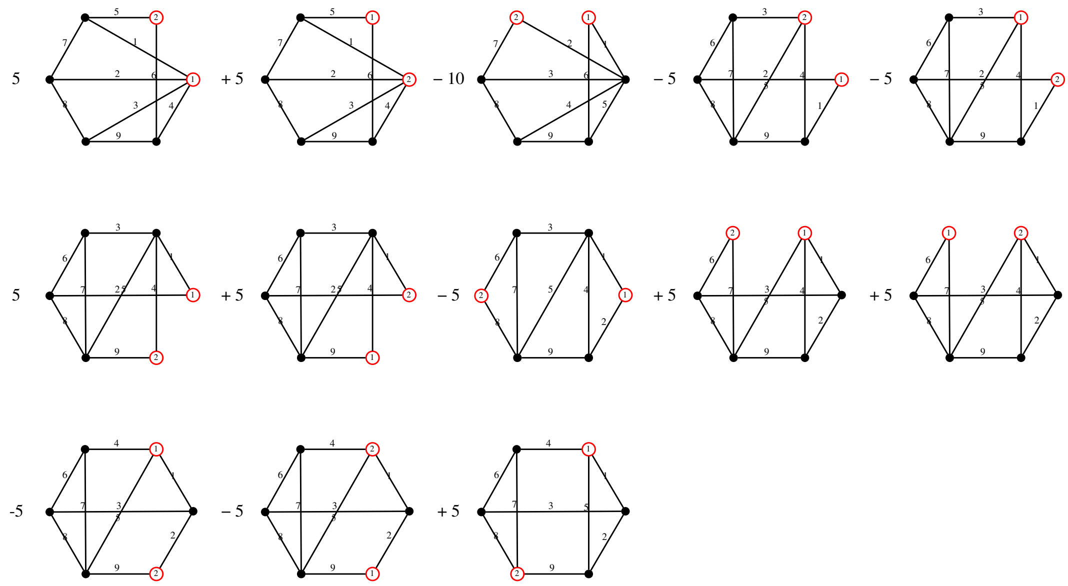

Figure 12: The element γ_2

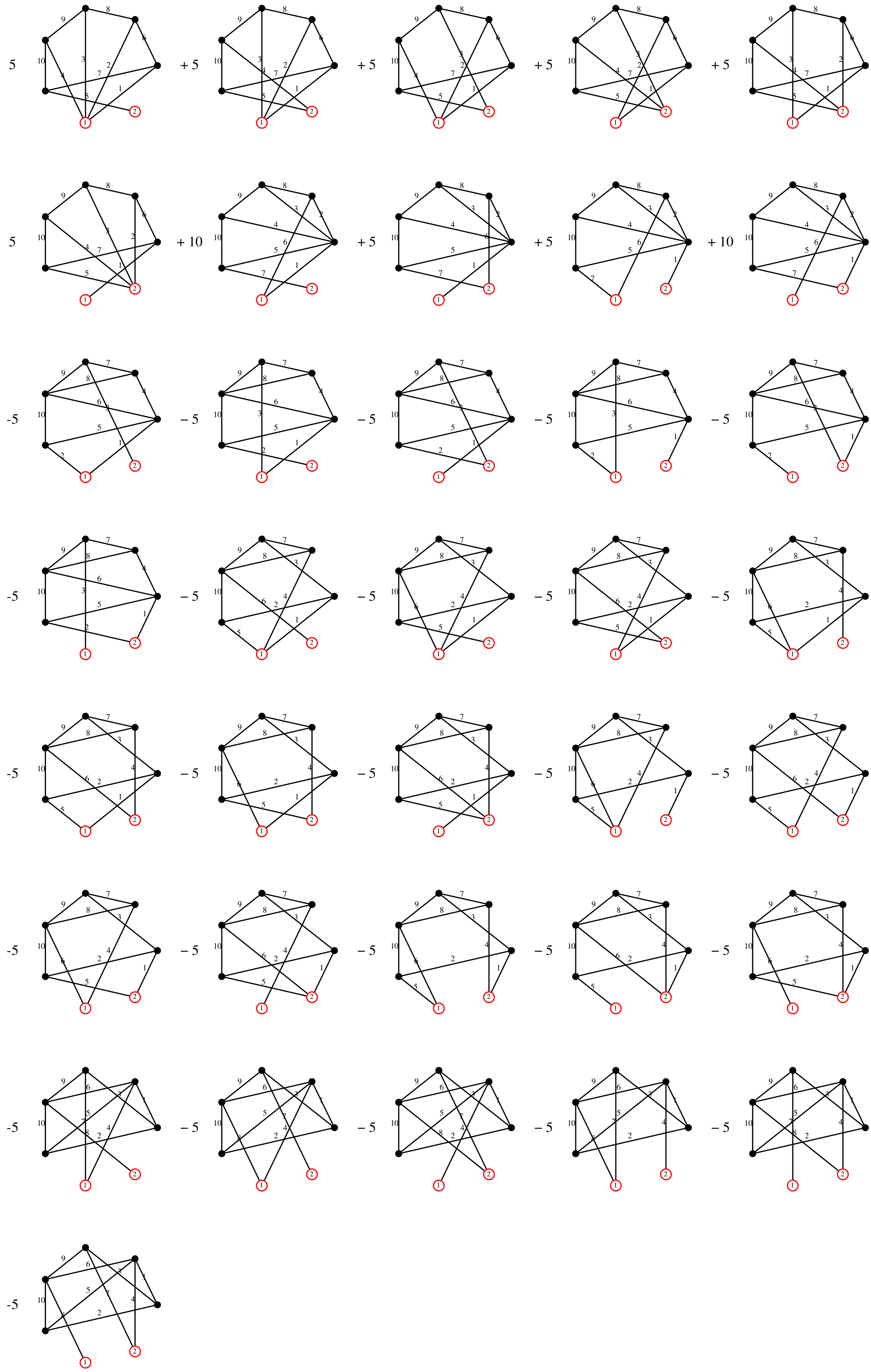

Figure 13: The element γ_2'

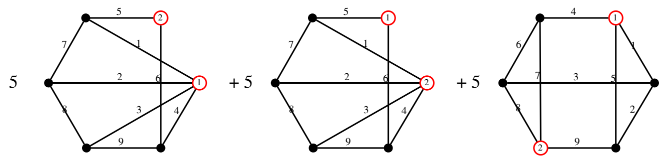

Figure 14: The element T

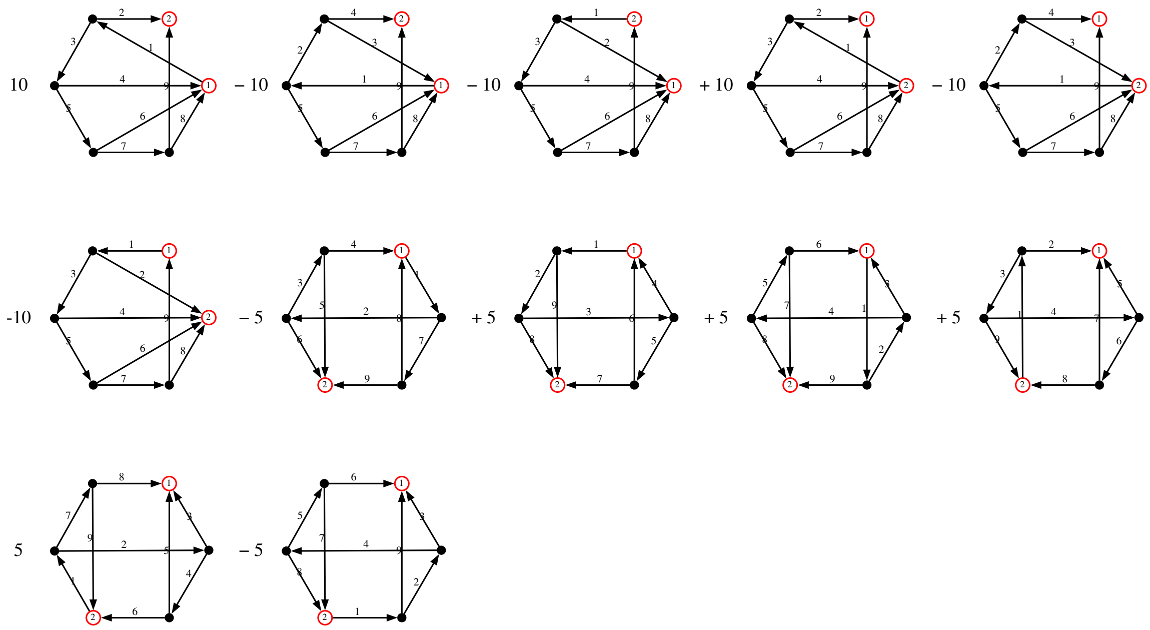

Figure 15: The element in $\mathfrak{tder}_2$

B The seven wheel under the map ϕ

In [9] the authors give a description of a heptagon-wheel cocycle, i.e. a cocycle containing the seven wheel. A graphical description of this cocycle can be found in [9] in Appendix A or here in Figure 17. Due to the size of γ_1, γ_2' and γ_2 they are not being displayed here. However, in Figure 16 the element T obtained in step 5 is depicted. Finally, the element σ_7 in $\mathfrak{grt}_1$ corresponding to the heptagon-wheel cocycle is given by

$$\begin{aligned}
\sigma_7 := {} & 14 \cdot [Y,[Y,[Y,[Y,[Y,[Y,X]]]]]] - 42 \cdot [Y,[Y,[Y,[Y,[[Y,X],X]]]]] \\
& + 70 \cdot [Y,[Y,[[Y,[Y,X]],[Y,X]]]] + 70 \cdot [Y,[Y,[Y,[[[Y,X],X],X]]]] \\
& - 28 \cdot [[Y,[Y,[Y,X]]],[Y,[Y,X]]] + \frac{133}{8} \cdot [Y,[Y,[[Y,X],[[Y,X],X]]]] \\
& - \frac{1211}{8} \cdot [Y,[[Y,[[Y,X],X]],[Y,X]]] - 70 \cdot [Y,[Y,[[[[Y,X],X],X],X]]] \\
& - 28 \cdot [[Y,[Y,X]],[Y,[[Y,X],X]]] + \frac{119}{8} \cdot [[[Y,[Y,X]],[Y,X]],[Y,X]] \\
& - \frac{693}{8} \cdot [Y,[[Y,X],[[[Y,X],X],X]]] + \frac{427}{8} \cdot [[Y,[[Y,X],X]],[[Y,X],X]] \\
& + \frac{763}{8} \cdot [[Y,[[[Y,X],X],X]],[Y,X]] + 42 \cdot [Y,[[[[[Y,X],X],X],X],X]] \\
& - \frac{455}{8} \cdot [[Y,X],[[Y,X],[[Y,X],X]]] + 56 \cdot [[Y,X],[[[[Y,X],X],X],X]] \\
& + 42 \cdot [[[Y,X],X],[[[Y,X],X],X]] - 14 \cdot [[[[[[Y,X],X],X],X],X],X].
\end{aligned}$$

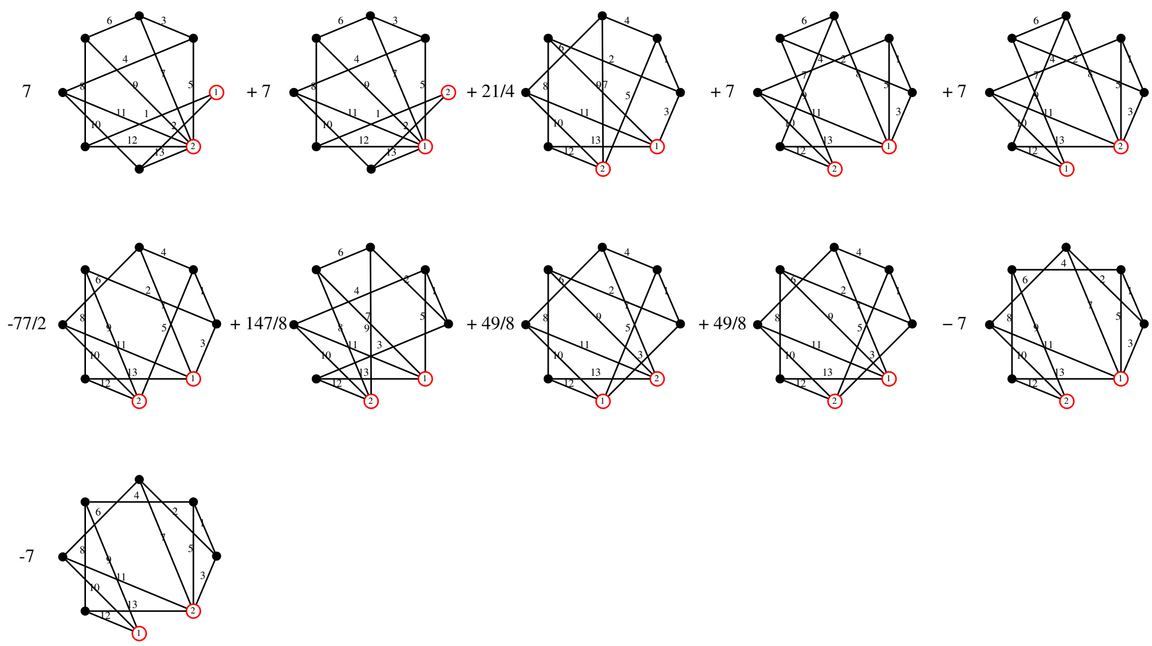

Figure 16: The element T

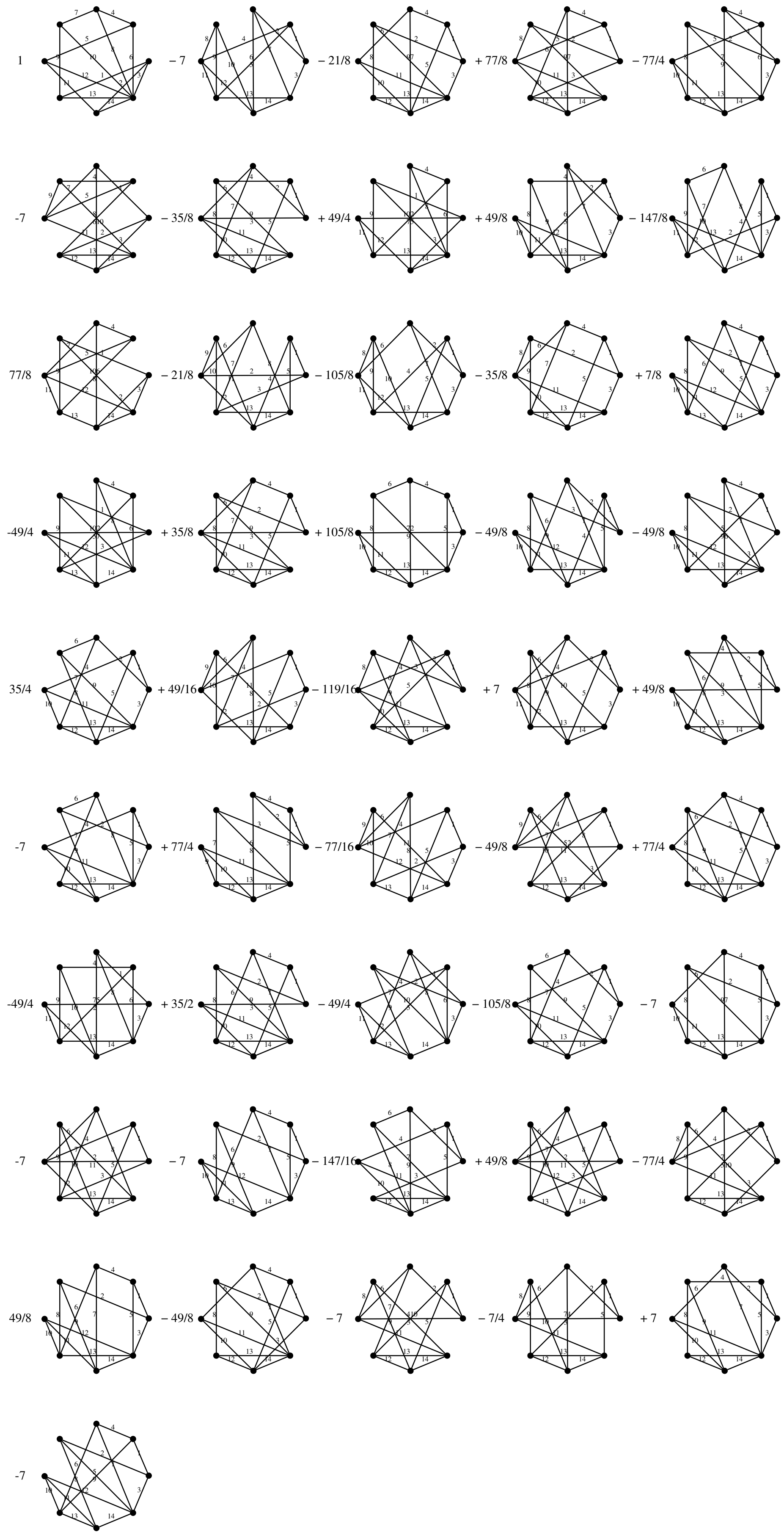

Figure 17: The heptagon-wheel cocycle.

C Python implementation

The code of the Python implementation can be found on github under `github.com/jlportner/MscArbeitProgramming`. It is structured into two parts the folder `GraphComputations` contains the implementation of the map ϕ and the graph complexes `GC` and `graphs`. Examples on how to use these can be found in the file `sevenwheel.py` and `fiveWheel.py` which create the images in Appendix A and B respectively.

The second folder `TauComputations` contains the implementation of calculating the $c_{\alpha,\beta}, c_{\alpha,\beta,\gamma}$ and then using those to give elements in depth 3 of Φ^t and Φ_{AT}. Moreover, it is used to generate the definitions for σ_9, σ_{11} and σ_{13}. A small working example on how to get the coefficients $c_{\alpha,\beta}, c_{\alpha,\beta,\gamma}$ and Φ_{AT} can be found in the file `main.py`.

Finally, the code has quite a few dependencies:

- `sagemath` needs to be installed,
- `maple` needs to be installed,
- `graphviz` needs to be installed,
- the python packages `numpy`, `networkx` and `pydot` need to be available,
- the maple package `HyperlogProcedures` by Oliver Schnetz (`https://www.math.fau.de/person/oliver-schnetz/`) needs to be on the computer and its path needs to be set in the function `startHyperlogProc()`.

D The values of the depth 3 coefficients $c_{\alpha,\beta,\gamma}$

n=3

$$c_{1,1,2} = \frac{195195 i\,\zeta(7)}{256\,\pi^7} \qquad c_{2,0,2} = \frac{183183 i\,\zeta(7)}{256\,\pi^7} \qquad c_{0,1,3} = \frac{297297 i\,\zeta(7)}{256\,\pi^7}$$
$$c_{1,0,3} = \frac{327327 i\,\zeta(7)}{256\,\pi^7} \qquad c_{0,0,4} = \frac{15015 i\,\zeta(7)}{16\,\pi^7}$$

n=4

$$c_{1,2,3} = -\frac{2686255 i\,\zeta(9)}{256\,\pi^9} \qquad c_{2,1,3} = -\frac{19606015 i\,\zeta(9)}{512\,\pi^9} \qquad c_{3,0,3} = -\frac{5676385 i\,\zeta(9)}{512\,\pi^9}$$
$$c_{0,2,4} = -\frac{10149425 i\,\zeta(9)}{512\,\pi^9} \qquad c_{1,1,4} = -\frac{33098065 i\,\zeta(9)}{1024\,\pi^9} \qquad c_{2,0,4} = -\frac{21623745 i\,\zeta(9)}{1024\,\pi^9}$$
$$c_{0,1,5} = -\frac{22401665 i\,\zeta(9)}{1024\,\pi^9} \qquad c_{1,0,5} = -\frac{14792635 i\,\zeta(9)}{1024\,\pi^9} \qquad c_{0,0,6} = -\frac{255255 i\,\zeta(9)}{32\,\pi^9}$$

n=5

Let

$$e_1 := 116396280 \cdot \frac{\zeta(11)}{(2\pi i)^{11}}$$
$$e_2 := \frac{7759752}{5} \cdot \frac{\zeta_{\mathrm{sv}}(5,3,3)}{(2\pi i)^{11}} + 9618336\frac{\zeta(5)\zeta(3)^2}{(2\pi i)^{11}}$$

then

$$c_{3,2,3} = \frac{2701}{360}\,e_1 \qquad c_{1,3,4} = \frac{8519}{720}\,e_1 - 5\,e_2 \qquad c_{2,2,4} = \frac{9881}{240}\,e_1 - \frac{25}{2}\,e_2$$
$$c_{3,1,4} = \frac{5581}{720}\,e_1 + 5\,e_2 \qquad c_{4,0,4} = -\frac{139}{80}\,e_1 + \frac{5}{2}\,e_2 \qquad c_{0,3,5} = -\frac{3077}{720}\,e_1 + 5\,e_2$$
$$c_{1,2,5} = \frac{11717}{600}\,e_1 - 3\,e_2 \qquad c_{2,1,5} = \frac{13359}{400}\,e_1 - 9\,e_2 \qquad c_{3,0,5} = \frac{1757}{450}\,e_1 + e_2$$
$$c_{0,2,6} = -\frac{5063}{3600}\,e_1 + \frac{9}{2}\,e_2 \qquad c_{1,1,6} = \frac{55237}{3600}\,e_1 - 3\,e_2 \qquad c_{2,0,6} = \frac{571}{60}\,e_1 - \frac{5}{2}\,e_2$$
$$c_{0,1,7} = \frac{7651}{3600}\,e_1 + e_2 \qquad c_{1,0,7} = \frac{15869}{3600}\,e_1 - e_2 \qquad c_{0,0,8} = e_1$$

n=6

Let

$$f_1 := 2974571600 \cdot \frac{\zeta(13)}{(2\pi i)^{13}}$$
$$f_2 := 13520780 \cdot \frac{\zeta_{\mathrm{sv}(5,5,3)}}{(2\pi i)^{13}} - 485401000 \cdot \frac{\zeta(5)^2\zeta(3)}{(2\pi i)^{13}}$$
$$f_3 := 19315400 \cdot \frac{\zeta_{\mathrm{sv}}(7,3,3)}{(2\pi i)^{13}} - 832116000 \cdot \frac{\zeta(5)^2\zeta(3)}{(2\pi i)^{13}} + 321120800 \cdot \frac{\zeta(7)\zeta(3)^2}{(2\pi i)^{13}}$$

then

$$c_{3,3,4} = \frac{29023}{660}\,f_1 + 34\,f_2 - \frac{35}{2}\,f_3 \qquad c_{4,2,4} = \frac{9949}{220}\,f_1 + f_2$$
$$c_{1,4,5} = -\frac{762}{275}\,f_1 + \frac{188}{5}\,f_2 - \frac{35}{2}\,f_3 \qquad c_{2,3,5} = \frac{38889}{550}\,f_1 + \frac{532}{5}\,f_2 - 56\,f_3$$
$$c_{3,2,5} = \frac{2383}{25}\,f_1 + \frac{238}{5}\,f_2 - \frac{49}{2}\,f_3 \qquad c_{4,1,5} = \frac{13697}{275}\,f_1 - \frac{78}{5}\,f_2 + \frac{21}{2}\,f_3$$
$$c_{5,0,5} = \frac{5263}{1100}\,f_1 - \frac{28}{5}\,f_2 + \frac{7}{2}\,f_3 \qquad c_{0,4,6} = -\frac{1909}{300}\,f_1 - \frac{27}{5}\,f_2 + 7\,f_3$$
$$c_{1,3,6} = \frac{49439}{1650}\,f_1 + \frac{244}{5}\,f_2 - 21\,f_3 \qquad c_{2,2,6} = \frac{107601}{1100}\,f_1 + \frac{444}{5}\,f_2 - 49\,f_3$$
$$c_{3,1,6} = \frac{15773}{275}\,f_1 + \frac{98}{5}\,f_2 - \frac{21}{2}\,f_3 \qquad c_{4,0,6} = \frac{115}{11}\,f_1 - 5\,f_2 + \frac{7}{2}\,f_3$$
$$c_{0,3,7} = -\frac{4121}{3300}\,f_1 - \frac{58}{5}\,f_2 + \frac{21}{2}\,f_3 \qquad c_{1,2,7} = \frac{144101}{3850}\,f_1 + \frac{888}{35}\,f_2 - 12\,f_3$$
$$c_{2,1,7} = \frac{105194}{1925}\,f_1 + \frac{1144}{35}\,f_2 - 20\,f_3 \qquad c_{3,0,7} = \frac{12503}{924}\,f_1 + \frac{30}{7}\,f_2 - \frac{5}{2}\,f_3$$
$$c_{0,2,8} = \frac{33619}{7700}\,f_1 - \frac{239}{35}\,f_2 + \frac{11}{2}\,f_3 \qquad c_{1,1,8} = \frac{328863}{15400}\,f_1 + \frac{286}{35}\,f_2 - 5\,f_3$$
$$c_{2,0,8} = \frac{1063}{88}\,f_1 + 5\,f_2 - \frac{7}{2}\,f_3 \qquad c_{0,1,9} = \frac{174721}{46200}\,f_1 - \frac{46}{35}\,f_2 + f_3$$
$$c_{1,0,9} = \frac{219029}{46200}\,f_1 + \frac{46}{35}\,f_2 - f_3 \qquad c_{0,0,10} = f_1$$

n=7

Let

$$g_1 := 70578471600 \cdot \frac{\zeta(15)}{(2\pi i)^{15}}$$

$$g_2 := 258529200 \cdot \frac{\zeta_{\mathrm{sv}}(9,3,3)}{(2\pi i)^{15}} - 12409401600 \cdot \frac{\zeta(5)^3}{(2\pi i)^{15}} - 60512425440 \cdot \frac{\zeta(7)\zeta(5)\zeta(3)}{(2\pi i)^{15}} + 8056882080 \cdot \frac{\zeta(9)\zeta(3)^2}{(2\pi i)^{15}}$$

$$g_3 := \frac{1706292720}{7} \cdot \frac{\zeta_{\mathrm{sv}}(7,3,5)}{(2\pi i)^{15}} + 13650341760 \cdot \frac{\zeta(5)^3}{(2\pi i)^{15}} + 63728237760 \cdot \frac{\zeta(7)\zeta(5)\zeta(3)}{(2\pi i)^{15}}.$$

then

$$c_{3,4,5} = \frac{10077611}{5460} g_1 - 112 g_2 - \frac{3115}{22} g_3 \qquad c_{4,3,5} = \frac{21839549}{10920} g_1 - 98 g_2 - \frac{2765}{22} g_3$$

$$c_{5,2,5} = \frac{1127211}{4550} g_1 - \frac{63}{22} g_3 \qquad c_{1,5,6} = \frac{100099067}{109200} g_1 - 56 g_2 - 77 g_3$$

$$c_{2,4,6} = \frac{81750661}{21840} g_1 - 224 g_2 - \frac{6335}{22} g_3 \qquad c_{3,3,6} = \frac{948907}{240} g_1 - 224 g_2 - \frac{3115}{11} g_3$$

$$c_{4,2,6} = \frac{10459307}{7280} g_1 - 63 g_2 - \frac{1785}{22} g_3 \qquad c_{5,1,6} = -\frac{21282517}{109200} g_1 + 28 g_2 + \frac{679}{22} g_3$$

$$c_{6,0,6} = -\frac{1800467}{21840} g_1 + 7 g_2 + \frac{175}{22} g_3 \qquad c_{0,5,7} = -\frac{14737889}{109200} g_1 + 14 g_2 + \frac{203}{22} g_3$$

$$c_{1,4,7} = \frac{79501151}{50960} g_1 - 84 g_2 - \frac{1335}{11} g_3 \qquad c_{2,3,7} = \frac{609621581}{152880} g_1 - 232 g_2 - 295 g_3$$

$$c_{3,2,7} = \frac{132189913}{50960} g_1 - 144 g_2 - \frac{1965}{11} g_3 \qquad c_{4,1,7} = \frac{4842731}{10192} g_1 - 18 g_2 - \frac{255}{11} g_3$$

$$c_{5,0,7} = -\frac{59071547}{764400} g_1 + 8 g_2 + \frac{197}{22} g_3 \qquad c_{0,4,8} = -\frac{18460019}{76440} g_1 + 23 g_2 + \frac{205}{11} g_3$$

$$c_{1,3,8} = \frac{87199667}{76440} g_1 - 59 g_2 - \frac{925}{11} g_3 \qquad c_{2,2,8} = \frac{107067939}{50960} g_1 - \frac{243}{2} g_2 - \frac{3285}{22} g_3$$

$$c_{3,1,8} = \frac{130626607}{152880} g_1 - 47 g_2 - \frac{1235}{22} g_3 \qquad c_{4,0,8} = \frac{113563}{1560} g_1 - \frac{5}{2} g_2 - \frac{35}{11} g_3$$

$$c_{0,3,9} = -\frac{1760716}{9555} g_1 + 17 g_2 + \frac{335}{22} g_3 \qquad c_{1,2,9} = \frac{37359233}{76440} g_1 - 25 g_2 - \frac{365}{11} g_3$$

$$c_{2,1,9} = \frac{7076711}{11760} g_1 - 35 g_2 - \frac{445}{11} g_3 \qquad c_{3,0,9} = \frac{131597}{1040} g_1 - 7 g_2 - \frac{175}{22} g_3$$

$$c_{0,2,10} = -\frac{52070947}{764400} g_1 + \frac{13}{2} g_2 + \frac{137}{22} g_3 \qquad c_{1,1,10} = \frac{101249003}{764400} g_1 - 7 g_2 - \frac{89}{11} g_3$$

$$c_{2,0,10} = \frac{55641}{728} g_1 - \frac{9}{2} g_2 - \frac{105}{22} g_3 \qquad c_{0,1,11} = -\frac{5756327}{764400} g_1 + g_2 + g_3$$

$$c_{1,0,11} = \frac{13795127}{764400} g_1 - g_2 - g_3 \qquad c_{0,0,12} = g_1$$

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