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# EXPLICIT ASSOCIATOR RELATIONS FOR MULTIPLE ZETA VALUES

ISMAEL SOUDÈRES

ABSTRACT. Associators were introduced by Drinfel'd in [Dri91] as a monodromy representation of a Knizhnik-Zamolodchikov equation. Associators can be briefly described as formal series in two non-commutative variables satisfying three equations. These three equations yield a large number of algebraic relations between the coefficients of the series, a situation which is particularly interesting in the case of the original Drinfel'd associator, whose coefficients are multiple zetas values. In the first part of this paper, we work out these algebraic relations among multiple zeta values by direct use of the defining relations of associators. While well-known for the first two relations, the algebraic relations we obtain for the third (pentagonal) relation, which are algorithmically explicit although we do not have a closed formula, do not seem to have been previously written down. The second part of the paper shows that if one has an explicit basis for the bar-construction of the moduli space  $\mathcal{M}_{0,5}$  of genus zero Riemann surfaces with 5 marked points at one's disposal, then the task of writing down the algebraic relations corresponding to the pentagon relation becomes significantly easier and more economical compared to the direct calculation above. We discuss the explicit basis described by Brown and Gangl, which is dual to the basis of the enveloping algebra of the braids Lie algebra,  $U\mathfrak{B}_5$ .

In order to write down the relation between multiple zeta values, we then remark that it is enough to write down the relations associated to elements that generate the bar construction as an algebra. This corresponds to looking at the bar construction modulo shuffle, which is dual to the Lie algebra of 5-strand braids. We write down, in the appendix, the associated algebraic relations between multiple zeta values in weights 2 and 3.

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## 1. INTRODUCTION

In the first part of this introduction we recall the necessary definitions concerning associators, and in the second part, we recall the definitions and main result concerning multiple zeta values. In the third part, we give the outline of the paper and state the main results.

**1.1. Associators.** Let  $k$  be a field of characteristic 0. Let  $U\mathfrak{F}_2 = k\langle\langle X_0, X_1 \rangle\rangle$  be the ring of formal series over  $k$  in two non-commutative variables. The coproduct  $\Delta$  on  $U\mathfrak{F}_2$  is defined by

$$\Delta(X_0) = X_0 \otimes 1 + 1 \otimes X_0 \quad \Delta(X_1) = X_1 \otimes 1 + 1 \otimes X_1.$$

An element  $\Phi = \Phi(X_0, X_1) \in U\mathfrak{F}_2$  is *group-like* if it satisfies  $\Delta(\Phi) = \Phi \hat{\otimes} \Phi$  where  $\hat{\otimes}$  denotes the complete tensor product.

*Remark 1.1.* We remark that the constant term of a group-like element is 1.

**Definition 1.2.** If  $S$  is a finite set, let  $S^*$  denote the set of words with letters in  $S$ , that is the dictionary over  $S$ . If  $S = \{s_1, \dots, s_n\}$  we may write,  $\{s_1, \dots, s_n\}^*$ .

Let  $\mathcal{W}_{0,1}$  be the dictionary over  $\{X_0, X_1\}$ .

We remark that the monomial in  $U\mathfrak{F}_2$  are words in  $\mathcal{W}_{0,1}$ ; the empty word  $\emptyset$  in  $\mathcal{W}_{0,1}$  will be 1 by convention when considered in  $U\mathfrak{F}_2$ . The following definition allows us to define a filtration on  $U\mathfrak{F}_2$ .

**Definition 1.3.** The depth  $dp(W)$  of a monomial  $W \in U\mathfrak{F}_2$ , that is an element of  $\mathcal{W}_{0,1}$ , is the number of  $X_1$ , and its weight (or length)  $wt(W) = |W|$  is the number of letters.

The algebra  $U\mathfrak{F}_2$  is filtered by the weight, and its graded pieces of weight  $d$  are the subspaces generated by the monomial of length  $d$ ;  $U\mathfrak{F}_2$  is thus a graded algebra.

Let  $U\mathfrak{B}_5$  be the enveloping algebra of  $\mathfrak{B}_5$ , the completion (with respect to the natural grading) of the pure sphere braid Lie algebra; that is,  $U\mathfrak{B}_5$  is the quotient of  $C\langle\langle X_{ij} \rangle\rangle$  with  $1 \leq i \leq 5$  and  $1 \leq j \leq 5$  by the relations

- $X_{ii} = 0$  for  $1 \leq i \leq 5$ ,
- $X_{ij} = X_{ji}$  for  $1 \leq i, j \leq 5$ ,
- $\sum_{j=1}^5 X_{ij} = 0$  for  $1 \leq i \leq 5$ ,
- $[X_{ij}, X_{kl}] = 0$  if  $\{i, j\} \cap \{k, l\} = \emptyset$ .

**Definition 1.4** (Drinfel'd [Dri91]). A group-like element  $\Phi$  in  $U\mathfrak{F}_2$ , with zero coefficient in degree 1, together with a  $\mu \in k^*$  is an associator if it satisfies the following equations

$$(I) \quad \Phi(X_0, X_1)\Phi(X_1, X_0) = 1$$

$$(II) \quad e^{\frac{\mu}{2}X_0}\Phi(X_\infty, X_0)e^{\frac{\mu}{2}X_\infty}\Phi(X_1, X_\infty)e^{\frac{\mu}{2}X_1}\Phi(X_0, X_1) = 1 \quad \text{with } X_0 + X_1 + X_\infty = 0$$

$$(III) \quad \Phi(X_{12}, X_{23})\Phi(X_{34}, X_{45})\Phi(X_{51}, X_{12})\Phi(X_{23}, X_{34})\Phi(X_{45}, X_{51}) = 1 \quad \text{in } U\mathfrak{B}_5$$

We will write an associator as

$$\Phi(X_0, X_1) = \sum_{W \in \mathcal{W}_{0,1}} Z_W W = 1 + \sum_{\substack{W \in \mathcal{W}_{0,1} \\ W \neq \emptyset}} Z_W W,$$

as  $Z_\emptyset = 1$  because  $\Phi$  is group-like.

In [Dri91], Drinfel'd gives an explicit associator  $\Phi_{KZ}$  over  $\mathbb{C}$ , known as the Drinfel'd associator and associated to a Knizhnik-Zamolodchikov equation (KZ equation). More precisely, consider the KZ equation (see also [Fur03][§3]).

$$(KZ) \quad \frac{\partial g}{\partial u} = \left( \frac{X_0}{u} + \frac{X_1}{1-u} \right) \cdot g(u)$$

where  $g$  is an analytic function in one complex variable  $u$  with values in  $\mathbb{C}\langle\langle X_0, X_1 \rangle\rangle$  (analytic means that each coefficient is an analytic function). This equation has singularities only at 0, 1 and  $\infty$ . The equation (KZ) has a unique solution on  $C = \mathbb{C} \setminus (]-\infty, 0] \cup [1, \infty[)$  having a specified value at a given point in  $C$ , because  $C$  is simply connected. Moreover, at 0 (resp. 1), there exists a unique solution  $g_0(u)$  (resp.  $g_1(u)$ ) such that

$$g_0(u) \sim u^{X_0} \quad (u \rightarrow 0) \quad (\text{resp. } g_1(u) \sim (1-u)^{X_1} \quad (u \rightarrow 1)).$$

As  $g_0$  and  $g_1$  are invertible with specified asymptotic behavior, they must coincide up to multiplication on the right by an invertible element in  $\mathbb{C}\langle\langle X_0, X_1 \rangle\rangle$ .

**Definition 1.5.** The *Drinfel'd associator*<sup>1</sup>,  $\Phi_{KZ}$ , is the element in  $\mathbb{C}\langle\langle X_0, X_1 \rangle\rangle$  defined by

$$g_0(u) = g_1(u)\Phi_{KZ}(X_0, X_1).$$

In [Dri91], Drinfel'd proved the following result.

**Proposition 1.6.** *The element  $\Phi_{KZ}$  is a group-like element and it satisfies (I), (II) with  $\mu = 2i\pi$ , and (III) of definition 1.4. That is,*

$$(IKZ) \quad \Phi_{KZ}(X_0, X_1)\Phi_{KZ}(X_1, X_0) = 1$$

$$(II_{KZ}) \quad e^{i\pi X_0}\Phi_{KZ}(X_\infty, X_0)e^{i\pi X_\infty}\Phi_{KZ}(X_1, X_\infty)e^{i\pi X_1}\Phi_{KZ}(X_0, X_1) = 1 \\ \text{with } X_0 + X_1 + X_\infty = 0$$

$$(III_{KZ}) \quad \Phi_{KZ}(X_{12}, X_{23})\Phi_{KZ}(X_{34}, X_{45})\Phi_{KZ}(X_{51}, X_{12})\Phi_{KZ}(X_{23}, X_{34}) \\ \Phi_{KZ}(X_{45}, X_{51}) = 1 \quad \text{in } U\mathfrak{B}_5$$

**1.2. Multiple zeta values.** For a  $p$ -tuple  $\mathbf{k} = (k_1, \dots, k_p)$  of strictly positive integers with  $k_1 \geq 2$ , the multiple zeta value  $\zeta(\mathbf{k})$  is defined as

$$\zeta(\mathbf{k}) = \sum_{n_1 > \dots > n_p > 0} \frac{1}{n_1^{k_1} \dots n_p^{k_p}}.$$

**Definition 1.7.** The depth of a  $p$ -tuple of integers  $\mathbf{k} = (k_1, \dots, k_p)$  is  $dp(\mathbf{k}) = p$ , and its weight  $wt(\mathbf{k})$  is  $wt(\mathbf{k}) = k_1 + \dots + k_p$ .

To the tuple  $\mathbf{k}$ , with  $n = wt(\mathbf{k})$ , we associate the  $n$ -tuple:

$$\bar{\mathbf{k}} = \left( \underbrace{0, \dots, 0}_{k_1-1 \text{ times}}, 1, \dots, \underbrace{0, \dots, 0}_{k_p-1 \text{ times}}, 1 \right) = (\varepsilon_n, \dots, \varepsilon_1)$$

<sup>1</sup>In [Dri91], Drinfel'd actually defined  $\phi_{KZ}$  rather than  $\Phi_{KZ}$ , where  $\phi_{KZ}(X_0, X_1) = \Phi_{KZ}(\frac{1}{2i\pi}X_0, \frac{1}{2i\pi}X_1)$  and is defined via the KZ equation  $\frac{\partial g}{\partial u} = \frac{1}{2i\pi} \left( \frac{X_0}{u} + \frac{X_1}{1-u} \right) \cdot g(u)$

and the word in  $\{X_0, X_1\}^*$

$$X_{\varepsilon_n} \cdots X_{\varepsilon_1}.$$

This makes it possible to associate a multiple zeta value  $\zeta(W)$  to each word  $W$  in  $X_0\{X_0, X_1\}X_1$  (where  $W$  begins with  $X_0$  and ends with  $X_1$ ).

Following Kontsevich and Drinfel'd, one can write the multiple zeta values as a Chen iterated integral [Che73]

$$\zeta(\mathbf{k}) = \int_0^1 (-1)^p \frac{du}{u - \varepsilon_n} \circ \cdots \circ \frac{du}{u - \varepsilon_1}.$$

Note that, as  $k_1 \geq 2$ , we have  $\varepsilon_n = 0$ . This expression as an iterated integral leads directly to an expression of the multiple zeta values as an integral over a simplex

$$\zeta(\mathbf{k}) = \int_{\Delta_n} (-1)^p \frac{dt_1}{t_1 - \varepsilon_1} \wedge \cdots \wedge \frac{dt_n}{t_n - \varepsilon_n}$$

where  $\Delta_n = \{0 < t_1 < \cdots < t_n < 1\}$ .

Thanks to the work of Ecalle, Zagier, Ihara, Kaneko or Furusho we can extend the definition of multiple zeta values to tuples without the condition  $k_1 \geq 2$  (see [Rac02], [IKZ06] or [Fur03]). These extended multiple zeta values are called regularized multiple zeta values and we speak of regularizations. We will be interested in a specific regularization, the *shuffle regularization*.

**Definition 1.8** (Shuffle product). A shuffle of  $\{1, 2, \dots, n\}$  and  $\{1, \dots, m\}$  is a permutation  $\sigma$  of  $\{1, 2, \dots, n+m\}$  such that :

$$\sigma(1) < \sigma(2) < \cdots < \sigma(n) \quad \text{and} \quad \sigma(n+1) < \sigma(n+2) < \cdots < \sigma(n+m).$$

The set of all the shuffles of  $\{1, 2, \dots, n\}$  and  $\{1, \dots, m\}$  is denoted by  $\text{sh}(n, m)$

Let  $V = X_{i_1} \cdots X_{i_n}$  and  $W = X_{i_{n+1}} \cdots X_{i_{n+m}}$  be two words in  $\mathcal{W}_{0,1}$ . The shuffle of  $V$  and  $W$  is the collection of words

$$\text{sh}(V, W) = (X_{i_{\sigma^{-1}(1)}} X_{i_{\sigma^{-1}(2)}} \cdots X_{i_{\sigma^{-1}(n+m)}})_{\sigma \in \text{sh}(n, m)}.$$

Working in  $\mathbb{C}\langle\langle X_0, X_1 \rangle\rangle$ , we will also consider the sum

$$V \text{ III } W = \sum_{U \in \text{sh}(V, W)} U = \sum_{\sigma \in \text{sh}(n, m)} X_{i_{\sigma^{-1}(1)}} X_{i_{\sigma^{-1}(2)}} \cdots X_{i_{\sigma^{-1}(n+m)}}$$

and extend the shuffle product III by linearity.

**Definition 1.9.** The *shuffle regularization* of the multiple zeta values is the collection of real numbers  $(\zeta^{\text{III}}(W))_{W \in \mathcal{W}_{0,1}}$  such that:

- (1)  $\zeta^{\text{III}}(X_0) = \zeta^{\text{III}}(X_1) = 0$ ,
- (2)  $\zeta^{\text{III}}(W) = \zeta(W)$  for all  $W \in X_0 \mathcal{W}_{0,1} X_1$ ,
- (3)  $\zeta^{\text{III}}(V) \zeta^{\text{III}}(W) = \sum_{U \in \text{sh}(V, W)} \zeta^{\text{III}}(U)$  for all  $V, W \in \mathcal{W}_{0,1}$

These regularized multiple zeta values for words not in  $X_0 \mathcal{W}_{0,1} X_1$  are in fact linear combinations of the usual multiple zeta values, as has been shown explicitly by Furusho in [Fur03].

The coefficients of the Drinfel'd associator can be written in an explicit way using convergent multiple zeta values [Fur03].

**Proposition 1.10.** *Using the shuffle regularization we can write ([LM96], [Fur03])*

$$\Phi_{KZ}(X_0, X_1) = \sum_{W \in \mathcal{W}_{0,1}} (-1)^{\text{wt}(W)} \zeta^{\text{III}}(W) W.$$

**1.3. Main results.** In Theorem 2.2 and Theorem 2.8 we will give explicit relations between the coefficients of the series defining an associator  $\Phi$  equivalent to the relation (I) and (II) satisfied by  $\Phi$ . Both were well-known as it is easy to expand the product of the associators in  $U\mathfrak{F}_2$  even if the author do not know whether the relations of Theorem 2.8 have been written in the literature. In the case of the pentagon relation (III), writing down relations between the coefficients implies fixing a basis  $B$  of  $U\mathfrak{B}_5$ . Even if fixing such a basis breaks the natural symmetry of the pentagon relation (III), it is then possible to write a new family of relations between the coefficients of  $\Phi$  equivalent to (III<sub>KZ</sub>). More precisely, decomposing a word  $W$  in the letters  $X_{3,4}, X_{4,5}, X_{2,4}, X_{1,2}, X_{2,3}$  in the basis  $B$  we have

$$W = \sum_{b \in B} l_{b,W} b,$$

and we have the following theorem.

**Theorem** (Theorem 2.12). *The relation (III) is equivalent to the family of relations*

$$\forall b \in B \ (b \neq 1) \quad \sum_{W \in \{X_{3,4}, X_{4,5}, X_{2,4}, X_{1,2}, X_{2,3}\}^*} l_{b,W} C_{5,W} = 0$$

where the  $C_{5,W}$  are explicitly given by :

$$C_{5,W} = \sum_{\substack{U_1, \dots, U_5 \in W \\ U_1 \cdots U_5 = W}} Z_{\rho_1(U_1)} Z_{\rho_2(U_2)} Z_{\rho_3(U_3)} Z_{\rho_4(U_4)} Z_{\rho_5(U_5)}.$$

Applying this theorem to the particular basis  $B_4$  coming from the identification

$$U\mathfrak{B}_5 \simeq k\langle\langle X_{3,4}, X_{4,5}, X_{2,4} \rangle\rangle \rtimes k\langle\langle X_{1,2}, X_{2,3} \rangle\rangle,$$

one can compute the coefficients  $l_{b,W}$  using the equation defining  $U\mathfrak{B}_5$ . In particular it is easy to see that  $l_{b,W}$  is in  $\mathbb{Z}$  in that case.

After each family of relations between the coefficients, we apply our results to the particular case of the Drinfel'd associator and give the corresponding family between multiple zeta values ((3), (8) and (11)).

In Section 3 of the article, we explain how these families of relations between multiple zeta values are induced by iterated integrals on  $\mathcal{M}_{0,4}$  and  $\mathcal{M}_{0,5}$  using the bar construction studied by Brown in [Bro09]. The geometry of  $\mathcal{M}_{0,5}$  allows us in Proposition 3.15 to interpret the coefficients  $C_{5,W}$  using iterated integrals.

**Proposition** (Proposition 3.15). *For any bar symbol  $\omega_W$  dual to a word  $W$  in the letters  $X_{34}, X_{45}, X_{24}, X_{12}, X_{23}$ , we have*

$$C_{5,W} = \int_{\gamma} \text{Reg}(\omega_W, \gamma)$$

where  $\text{Reg}(\omega, D)$  is the regularisation of a bar symbol in  $\oplus \mathbb{H}^1(\mathcal{M}_{0,5})^{\otimes n}$  along boundary components  $D \subset \partial\mathcal{M}_{0,5}$ .

This is a consequence of Theorem 3.13 which links the family of relations (11) to the bar construction.

**Theorem** (Theorem 3.13). *The relation (III<sub>KZ</sub>) is equivalent to the family of relations*

$$\forall b_4 \in B_4 \quad \int_{\gamma} \text{Reg}(b_4^*, \gamma) = 0$$

which is exactly the family of relations (11). Here  $(b_4^*)_{b_4 \in B_4}$  denotes the basis in  $V(\mathcal{M}_{0,5})$ , the bar construction on  $\mathcal{M}_{0,5}$ , dual to the basis  $B_4$  of  $U\mathfrak{B}_5$  described earlier.

More generally, we then have that, for any basis  $F = (f)_{f \in F}$  on  $V(\mathcal{M}_{0,5})$ , the pentagon relation (III<sub>KZ</sub>) is equivalent to

$$\forall f \in F \quad \int_{\gamma} \text{Reg}(f, \gamma) = 0.$$

Brown, Gangl and Levin in [BGL10] obtain, using different methods and for another purpose, the same basis  $B_4^*$  of  $V(\mathcal{M}_{0,5})$  which is described there using combinatorial objects, that is the maximal triangulations of root decorated polygons.

Instead of looking all the elements of a basis  $F$  of  $V(\mathcal{M}_{0,5})$ , it is enough to consider only a subbasis that generates  $V(\mathcal{M}_{0,5})$  as a shuffle algebra. Indeed, if  $\omega$  in  $V(\mathcal{M}_{0,5})$  is equal to  $f_1 \sharp f_2$ , the iterated integral  $\int_{\gamma} \omega$  is equal to  $\int_{\gamma} f_1 \int_{\gamma} f_2$ . Thus it does not give a new relation between multiple zeta values. Considering a set of generators of the shuffle algebra leads to computing many less relations. In degree 2 and 3 we have respectively 4 and 10 generators instead of 19 and 65 elements in the vector space basis. In the appendix, we will give these relations in degree 2 and 3 using the basis  $B_4$ .

The multiplicative generators that we have found dont have a particularly simple expression in terms of symbols  $\omega_W$  dual to words  $W$  in the letters  $X_{34}, X_{45}, X_{24}, X_{12}, X_{23}$ . But it seems to be linked with our particular choice of indentification. The identification

$$U\mathfrak{B}_5 \simeq k\langle\langle X_{3,4}, X_{1,4}, X_{2,4} \rangle\rangle \rtimes k\langle\langle X_{1,2}, X_{2,3} \rangle\rangle$$

leads to another basis  $\tilde{B}_4$  of  $U\mathfrak{B}_5$ . Then, multiplicative generators can be found with a particularly simple expression in terms of symbols  $\omega_W$  dual to words  $W$  in the letters  $X_{34}, X_{14}, X_{24}, X_{12}, X_{23}$ . More precisely, writing such a word  $W$  as

$$W = \sum_{\tilde{b}_4 \in \tilde{B}_4} l_{\tilde{b}_4, W} \tilde{b}_4,$$

we can write  $\tilde{b}_4^* = \sum_W l_{\tilde{b}_4, W} \omega_W$ . The generators are elements  $\tilde{b}_4^*$  such that the number of  $l_{\tilde{b}_4, W}$  is as minimal as possible. This seems to be a general fact.

## 2. COMBINATORIAL DESCRIPTION OF ASSOCIATORS RELATIONS

The goal of this section is, for any associator and for the particular case of  $\Phi_{KZ}$ , to give an explicit expression for the relations between the coefficients derived from the associator relations (I), (II) and (III). For each of these relations, we will first study the case of a general associator and then deduce, for the Drinfel'd associator, relations between the regularized multiple zeta values. Let

$$\Phi = \sum_{W \in \mathcal{W}_{0,1}} Z_W W$$

be an associator. The idea will be to expand the product in the right hand side of the equations (I), (II) and (III) in a suitable basis of the space  $U\mathfrak{F}_2$  or  $U\mathfrak{B}_5$ .

**2.1. The symmetry, (I) and (I<sub>KZ</sub>).** Let  $P_2$  be the product  $\Phi(X_0, X_1)\Phi(X_1, X_0)$ . As the monomials in  $U\mathfrak{F}_2$ , that is words in  $\mathcal{W}_{0,1}$ , form a basis of  $U\mathfrak{F}_2$ , we can write  $P_2$  as

$$P_2 = \sum_{W \in \mathcal{W}_{0,1}} C_{2,W} W = 1 + \sum_{W \in \mathcal{W}_{0,1}, W \neq \emptyset} C_{2,W} W.$$

The relation (I) tells us that for each  $W \in \mathcal{W}_{0,1}$ ,  $W$  nonempty, we have

$$(1) \quad C_{2,W} = 0.$$

**Example 2.1.** In low degree we have the following relations:

- In degree one, there are just 2 words :  $X_0$  and  $X_1$  and (1) gives:

$$\begin{aligned} C_{2,X_0} &= Z_{X_0} + Z_{X_1} = 0 \\ C_{2,X_1} &= Z_{X_1} + Z_{X_0} = 0 \end{aligned}$$

- In degree two there are 4 words  $X_0X_0$ ,  $X_0X_1$ ,  $X_1X_0$  and  $X_1X_1$  and (1) gives:

$$\begin{aligned} C_{2,X_0X_0} &= Z_{X_0X_0} + Z_{X_0}Z_{X_1} + Z_{X_1}X_1 = 0 \\ C_{2,X_0X_1} &= Z_{X_0X_1} + Z_{X_0}Z_{X_0} + Z_{X_1}X_0 = 0 \\ C_{2,X_1X_0} &= Z_{X_1X_0} + Z_{X_1}Z_{X_1} + Z_{X_0}X_1 = 0 \\ C_{2,X_1X_1} &= Z_{X_1X_1} + Z_{X_1}Z_{X_0} + Z_{X_0}X_0 = 0 \end{aligned}$$

- In degree three there are 8 words. Looking at the coefficients of the words  $X_0X_0X_1$  in  $P_2$ , equation (1) gives:

$$Z_{X_0X_0X_1} + Z_{X_0X_0}Z_{X_0} + Z_{X_0}Z_{X_1X_0} + Z_{X_1X_1X_0} = 0$$

Let  $\theta$  be the automorphism of  $U\mathfrak{F}_2$  that sends  $X_0$  to  $X_1$  and  $X_1$  to  $X_0$ . Then we have:

**Theorem 2.2.** *The relation (I) is equivalent to the family of relations*

$$(2) \quad \forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\}, \quad \sum_{\substack{U_1, U_2 \in \mathcal{W}_{0,1} \\ U_1 U_2 = W}} Z_{U_1} Z_{\theta(U_2)} = 0.$$

*Proof.* As  $\Phi(X_1, X_0) = \theta(\Phi(X_0, X_1))$ , we have

$$\begin{aligned} \Phi(X_1, X_0) &= \theta \left( 1 + \sum_{\substack{W \in \mathcal{W}_{0,1} \\ W \neq \emptyset}} Z_W W \right) = 1 + \sum_{\substack{W \in \mathcal{W}_{0,1} \\ W \neq \emptyset}} Z_W \theta(W) \\ &= 1 + \sum_{\substack{W \in \mathcal{W}_{0,1} \\ W \neq \emptyset}} Z_{\theta(W)} W. \end{aligned}$$

Then, expanding the product  $P_2$  and reorganizing, we have

$$\begin{aligned} \Phi(X_0, X_1) \Phi(X_1, X_0) &= \left( 1 + \sum_{\substack{U_1 \in \mathcal{W}_{0,1} \\ U_1 \neq \emptyset}} Z_{U_1} U_1 \right) \left( 1 + \sum_{\substack{U_2 \in \mathcal{W}_{0,1} \\ U_2 \neq \emptyset}} Z_{\theta(U_2)} U_2 \right) \\ &= \sum_{\substack{W \in \mathcal{W}_{0,1} \\ W \neq \emptyset}} \left( \sum_{\substack{U_1, U_2 \in \mathcal{W}_{0,1} \\ U_1 U_2 = W}} Z_{U_1} Z_{\theta(U_2)} \right) W. \end{aligned}$$

□

**Corollary 2.3.** *The relation (I<sub>KZ</sub>) is equivalent to the family of relations*

$$(3) \quad \forall W \in \mathcal{W}_{0,1}, \quad \sum_{\substack{U_1, U_2 \in \mathcal{W}_{0,1} \\ U_1 U_2 = W}} (-1)^{dp(U_1)} \zeta^m(U_1) (-1)^{dp(\theta(U_2))} \zeta^m(\theta(U_2)) = 0,$$

*that family being equivalent to the following*

$$(4) \quad \forall W \in \mathcal{W}_{0,1}, \quad \sum_{\substack{U_1, U_2 \in \mathcal{W}_{0,1} \\ U_1 U_2 = W}} (-1)^{|U_2|} \zeta^m(U_1) \zeta^m(\theta(U_2)) = 0.$$



**2.2. The 3-cycle or the hexagon relation, (II) and (II<sub>KZ</sub>).** For any element  $P = \sum_{W \in \mathcal{W}_{0,1}} a_W W$  in  $U\mathfrak{F}_2$ , let  $C_{0,1}(P|W)$  be the coefficient  $a_W$  of the monomial  $W$ .

Let  $P_3$  be the product

$$P_3 = e^{\frac{\mu}{2}X_0}\Phi(X_\infty, X_0)e^{\frac{\mu}{2}X_\infty}\Phi(X_1, X_\infty)e^{\frac{\mu}{2}X_1}\Phi(X_0, X_1).$$

We can write  $P_3$  as

$$P_3 = \sum_{W \in \mathcal{W}_{0,1}} C_{0,1}(P_3|W)W = \sum_{W \in \mathcal{W}_{0,1}} C_{3,W}W.$$

The relation (II) tells us that for each  $W \in \mathcal{W}_{0,1}$ ,  $W \neq \emptyset$ , we have

$$(5) \quad C_{3,W} = 0.$$

In order to make these coefficients explicit, we will need some definitions.

**Definition 2.4.** Let  $\alpha_0$  (resp.  $\alpha_1$  and  $\alpha_\infty$ ) be the endomorphism of  $U\mathfrak{F}_2$  defined on  $X_0$  and  $X_1$  by :

$$\alpha_0(X_0) = X_0 \quad \text{and} \quad \alpha_0(X_1) = 0,$$

respectively

$$\alpha_1(X_0) = 0 \quad \text{and} \quad \alpha_1(X_1) = X_1$$

and

$$\alpha_\infty = -(\alpha_0 + \alpha_1).$$

Let  $\tilde{\alpha}_i$  be the composition of  $\alpha_i$  with  $X_0, X_1 \mapsto 1$ .

The following proposition is a consequence of the expression of the exponential

$$\forall P \in U\mathfrak{F}_2 \quad \exp(P) = \sum_{n \geq 0} \frac{P^n}{n!}$$

and of the equality

$$(6) \quad (-X_0 - X_1)^n = \sum_{\substack{W \in \mathcal{W}_{0,1} \\ |W|=n}} (-1)^{|W|} W.$$

**Proposition 2.5.** Let  $W$  be a word in  $\mathcal{W}_{0,1}$ , we have

$$\begin{aligned} C_{0,1}(e^{\frac{\mu}{2}X_0}|W) &= \frac{\mu^{|W|}}{2^{|W|}|W|!} \tilde{\alpha}_0(W), \\ C_{0,1}(e^{\frac{\mu}{2}X_1}|W) &= \frac{\mu^{|W|}}{2^{|W|}|W|!} \tilde{\alpha}_1(W) \quad \text{and} \\ C_{0,1}(e^{\frac{\mu}{2}X_\infty}|W) &= (-1)^{|W|} \frac{\mu^{|W|}}{2^{|W|}|W|!}. \end{aligned}$$

In order to describe the coefficient of  $\Phi(X_i, X_j)$ , with either one of the variables being  $X_\infty$ , we introduce a set of different decompositions of  $W$  into sub-words.

**Definition 2.6.** Let  $W$  be a word in  $\mathcal{W}_{0,1}$ . For  $i \in \{0, 1\}$ , let  $\text{dec}_{0,1}(W, X_i)$  be the set of tuples  $(V_1, X_i^{k_1}, V_2, X_i^{k_2}, \dots, V_p, X_i^{k_p})$  with  $1 \leq p < \infty$ ,  $V_j \in \mathcal{W}_{0,1}$  and  $V_2, \dots, V_p \neq \emptyset$  such that

$$W = V_1 X_i^{k_1} V_2 X_i^{k_2} \dots V_p X_i^{k_p}.$$

We will write  $(\mathbf{V}, \mathbf{k}) \in \text{dec}_{0,1}(W, X_i)$  instead of  $(V_1, X_i^{k_1}, V_2, X_i^{k_2}, \dots, V_p, X_i^{k_p}) \in \text{dec}_{0,1}(W, X_i)$  and  $|\mathbf{V}|$  (resp.  $|\mathbf{k}|$ ) will denote  $|V_1| + \dots + |V_p|$  (resp.  $k_1 + \dots + k_p$ ).

The following proposition describes the coefficient of  $W$  in the series  $\Phi(X_0, X_1)$ ,  $\Phi(X_\infty, X_0)$  and  $\Phi(X_1, X_\infty)$ .

**Proposition 2.7.** *Let  $W$  be a word in  $\mathcal{W}_{0,1}$ . We have*

$$C_{0,1}(\Phi(X_0, X_1)|W) = Z_W.$$

The coefficients  $C_{0,1}(\Phi(X_\infty, X_0)|W)$  and  $C_{0,1}(\Phi(X_1, X_\infty)|W)$  can be written as

$$C_{0,1}(\Phi(X_\infty, X_0)|W) = \sum_{(\mathbf{V}, \mathbf{k}) \in \text{deco}_{0,1}(W, X_0)} (-1)^{|\mathbf{V}|} Z_{X_0^{|\mathbf{V}_1|} X_1^{k_1} X_0^{|\mathbf{V}_2|} X_1^{k_2} \dots X_0^{|\mathbf{V}_p|} X_1^{k_p}}$$

and

$$C_{0,1}(\Phi(X_1, X_\infty)|W) = \sum_{(\mathbf{V}, \mathbf{k}) \in \text{deco}_{0,1}(W, X_1)} (-1)^{|\mathbf{V}|} Z_{X_1^{|\mathbf{V}_1|} X_0^{k_1} X_1^{|\mathbf{V}_2|} X_0^{k_2} \dots X_1^{|\mathbf{V}_p|} X_0^{k_p}}.$$

*Proof.* The first statement is immediate. Let  $\mathcal{L}_{2,c}(\mathbb{N})$  denote the set of double  $p$ -tuples ( $0 \leq p < \infty$ ) of integers  $((l_1, \dots, l_p), (k_1, \dots, k_p))$  with  $k_i, l_i \in \mathbb{N}$  and let  $(\mathbf{l}, \mathbf{k})$  denote an element of  $\mathcal{L}_{2,c}(\mathbb{N})$ . We can write  $\Phi(X_\infty, X_0)$  as

$$\Phi(X_\infty, X_0) = \sum_{(\mathbf{l}, \mathbf{k}) \in \mathcal{L}_{2,c}(\mathbb{N})} Z_{X_0^{l_1} X_1^{k_1} \dots X_0^{l_p} X_1^{k_p}} X_\infty^{l_1} X_0^{k_1} \dots X_\infty^{l_p} X_0^{k_p}$$

which equals

$$\sum_{(\mathbf{l}, \mathbf{k}) \in \mathcal{L}_{2,c}(\mathbb{N})} Z_{X_0^{l_1} X_1^{k_1} \dots X_0^{l_p} X_1^{k_p}} (-1)^{|\mathbf{l}|} (X_0 + X_1)^{l_1} X_0^{k_1} \dots (X_0 + X_1)^{l_p} X_0^{k_p}.$$

Reorganizing, we see that the expression of  $C_{0,1}(\Phi(X_\infty, X_0)|W)$  follows from (6); the case of  $C_{0,1}(\Phi(X_1, X_\infty)|W)$  is identical.  $\square$

**Theorem 2.8.** *The relation (II) is equivalent to the family of relations*

$$(7) \quad \forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\},$$

$$\sum_{\substack{W_1, \dots, W_6 \in \mathcal{W}_{0,1} \\ W_1 \dots W_6 = W}} \frac{\mu^{|W_1|}}{2^{|W_1|} |W_1|!} \tilde{\alpha}_0(W_1) \times \\ \left( \sum_{(\mathbf{U}, \mathbf{k}) \in \text{deco}_{0,1}(W_2, X_0)} (-1)^{|\mathbf{U}|} Z_{X_0^{|\mathbf{U}_1|} X_1^{k_1} \dots X_0^{|\mathbf{U}_p|} X_1^{k_p}} \right) (-1)^{|W_3|} \frac{\mu^{|W_3|}}{2^{|W_3|} |W_3|!} \times \\ \left( \sum_{(\mathbf{V}, \mathbf{l}) \in \text{deco}_{0,1}(W_4, X_1)} (-1)^{|\mathbf{V}|} Z_{X_1^{|\mathbf{V}_1|} X_0^{l_1} \dots X_1^{|\mathbf{V}_p|} X_0^{l_p}} \right) \frac{\mu^{|W_5|}}{2^{|W_5|} |W_5|!} \tilde{\alpha}_1(W_5) Z_{W_6} = 0.$$

*Proof.* The relation (II) is equivalent to the family of relations

$$\forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\} \quad C_{0,1}(P_3, W) = 0.$$

As  $P_3$  is a product of six factors, this is equivalent to

$$\forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\} \\ C_{0,1}(e^{\frac{\mu}{2} X_0}, W) C_{0,1}(\Phi(X_\infty, X_0), W) \cdot \\ C_{0,1}(e^{\frac{\mu}{2} X_\infty}, W) C_{0,1}(\Phi(X_1, X_\infty), W) \cdot \\ C_{0,1}(e^{\frac{\mu}{2} X_1}, W) C_{0,1}(\Phi(X_0, X_1), W) = 0.$$

The proposition follows, then, from Proposition 2.5 and 2.7.  $\square$

**Corollary 2.9.** *The relation  $(\text{II}_{\text{KZ}})$  is equivalent to the family of relations*

$$(8) \quad \forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\},$$

$$\sum_{\substack{W_1, \dots, W_6 \in \mathcal{W}_{0,1} \\ W_1 \cdots W_6 = W}} \frac{(i\pi)^{|W_1|}}{|W_1|!} \tilde{\alpha}_0(W_1) \times$$

$$\left( \sum_{\substack{(\mathbf{U}, \mathbf{k}) \\ \in \text{dec}_{0,1}(W_2, X_0)}} (-1)^{|W_2|} \zeta^{\mathfrak{m}}(X_0^{|\mathbf{U}_1|} X_1^{k_1} \cdots X_0^{|\mathbf{U}_p|} X_1^{k_p}) \right) (-1)^{|W_3|} \frac{(i\pi)^{|W_3|}}{|W_3|!} \times$$

$$\left( \sum_{\substack{(\mathbf{V}, \mathbf{l}) \\ \in \text{dec}_{0,1}(W_4, X_1)}} \zeta^{\mathfrak{m}}(X_1^{|\mathbf{V}_1|} X_0^{l_1} \cdots X_1^{|\mathbf{V}_p|} X_0^{l_p}) \right) \frac{(i\pi)^{|W_5|}}{|W_5|!} \tilde{\alpha}_1(W_5) (-1)^{d_p(W_6)} \zeta^{\mathfrak{m}}(W_6) = 0.$$

**2.3. The 5-cycle or the pentagon relation, (III) and  $(\text{III}_{\text{KZ}})$ .** In order to find families of relations between the coefficient equivalent to (I) and (II) we have decomposed the product  $P_2$  and  $P_3$  on a basis of  $U\mathfrak{F}_2$ , the words in  $X_0$  and  $X_1$ . We will do the same thing here but the monomial in the variable  $X_{ij}$  are not a linear basis of  $U\mathfrak{B}_5$  because there are relations between the  $X_{ij}$ . Using the relation defining  $U\mathfrak{B}_5$  we can see that  $X_{51} = -X_{12} - X_{13} - X_{14}$  and that

$$\begin{aligned} X_{51} &= -X_{54} - X_{53} - X_{52} \\ &= 2X_{23} + 2X_{24} + 2X_{34} + X_{12} + X_{13} + X_{14}. \end{aligned}$$

Then, as the characteristic of  $k$  is zero, we have  $X_{51} = X_{23} + X_{24} + X_{34}$ . In this section, we will expand the product in the R.H.S of III using this relation and then decompose this product on a linear basis of  $U\mathfrak{B}_5$ . Let  $B$  denote a linear basis of  $U\mathfrak{B}_5$  (with 1 being an element of  $B$ ) and  $B_4$  the basis of  $U\mathfrak{B}_5$  coming from the identification

$$U\mathfrak{B}_5 \simeq k\langle\langle X_{24}, X_{34}, X_{45} \rangle\rangle \rtimes k\langle\langle X_{12}, X_{23} \rangle\rangle.$$

This identification is induced by the morphism  $U\mathfrak{B}_5 \rightarrow U\mathfrak{F}_2$  that maps  $X_{i4}$  to 0 ( $1 \leq i \leq 5$ ),  $X_{12}$  to  $X_0$ ,  $X_{23}$  to  $X_1$ , the images of the other generators being easily deduce from those. The basis  $B_4$  is formed by 1 and the monomials, that is words,  $U_{245}V_{123}$  where  $U_{245}$  is a word in  ${}_{24}\mathcal{W}_{34,45} = \{X_{24}, X_{34}, X_{45}\}^*$  and  $V_{123}$  is in  $\mathcal{W}^{12,23} = \{X_{12}, X_{23}\}^*$ . Speaking of the empty word  $\emptyset$  in  $B_4$ , we will mean 1 when seen in  $U\mathfrak{B}_5$  and  $\emptyset$  when seen as the word.

Let  $\mathcal{W}$  be the dictionary  $\{X_{24}, X_{34}, X_{45}, X_{12}, X_{23}\}^*$ , and let  ${}_{24}\mathcal{W}_{34}^{23}$  and  ${}_{24}\mathcal{W}_{34}^{12,23}$  be respectively the sub-dictionary  $\{\tilde{X}_{23}, \tilde{X}_{24}, \tilde{X}_{34}\}^*$  and  $\{\tilde{X}_{12}, \tilde{X}_{23}, \tilde{X}_{24}, \tilde{X}_{34}\}^*$ .

Let  $P_5$  be the product in  $U\mathfrak{B}_5$ .

$$\Phi(X_{12}, X_{23})\Phi(X_{34}, X_{45})\Phi(X_{51}, X_{12})\Phi(X_{23}, X_{34})\Phi(X_{45}, X_{51}).$$

As  $X_{51} = X_{23} + X_{24} + X_{34}$ , we can write  $P_5$  without using  $X_{51}$

$$\begin{aligned} P_5 &= \Phi(X_{12}, X_{23})\Phi(X_{34}, X_{45})\Phi(X_{23} + X_{24} + X_{34}, X_{12})\Phi(X_{23}, X_{34}) \\ &\quad \Phi(X_{45}, X_{23} + X_{24} + X_{34}). \end{aligned}$$

Expanding the terms  $(X_{23} + X_{24} + X_{34})^n$  as

$$\sum_{\substack{W \in {}_{24}\mathcal{W}_{34}^{23} \\ |W|=n}} W,$$

we have

$$(9) \quad P_5 = \sum_{W \in \mathcal{W}} C_{5,W} W.$$

Despite that this writing is not unique as a decomposition of  $P_5$  in  $\mathcal{W}$ ; those  $C_{5,W}$  are the coefficients of a word  $W$  just after expanding the product  $P_5$  without  $X_{51}$  and as such are unique and well defined.

**Lemma 2.10.** *Let  $\rho_1, \rho_2, \rho_3, \rho_4, \rho_5$  be the morphisms from  $U\mathfrak{B}_5$  to  $U\mathfrak{F}_2$  defined respectively on the monomial  $X_{24}$  by,  $X_{34}, X_{45}, X_{12}, X_{23}$  as :*

$$\begin{aligned} \rho_1(X_{12}) &= X_0, & \rho_1(X_{23}) &= X_1, & \rho_1(X_{34}) &= 0, & \rho_1(X_{45}) &= 0, & \rho_1(X_{24}) &= 0, \\ \rho_2(X_{12}) &= 0, & \rho_2(X_{23}) &= 0, & \rho_2(X_{34}) &= X_0, & \rho_2(X_{45}) &= X_1, & \rho_2(X_{24}) &= 0, \\ \rho_3(X_{12}) &= X_1, & \rho_3(X_{23}) &= X_0, & \rho_3(X_{34}) &= X_0, & \rho_3(X_{45}) &= 0, & \rho_3(X_{24}) &= X_0, \\ \rho_4(X_{12}) &= 0, & \rho_4(X_{23}) &= X_0, & \rho_4(X_{34}) &= X_1, & \rho_4(X_{45}) &= 0, & \rho_4(X_{24}) &= 0, \\ \rho_5(X_{12}) &= 0, & \rho_5(X_{23}) &= X_1, & \rho_5(X_{34}) &= X_1, & \rho_5(X_{45}) &= X_0, & \rho_5(X_{24}) &= X_1. \end{aligned}$$

**Proposition 2.11.** *For all words  $W \in \mathcal{W}$  ( $W \neq \emptyset$ ), the coefficient  $C_{5,W}$  is given by*

$$(10) \quad C_{5,W} = \sum_{\substack{U_1, \dots, U_5 \in \mathcal{W} \\ U_1 \dots U_5 = W}} Z_{\rho_1(U_1)} Z_{\rho_2(U_2)} Z_{\rho_3(U_3)} Z_{\rho_4(U_4)} Z_{\rho_5(U_5)},$$

where by convention  $Z_0 = 0$ .

*Proof.* It is enough to show that the  $i$ -th factor of  $P_5$  without using  $X_{51}$  can be written as

$$\sum_{U_i \in \mathcal{W}} Z_{\rho_i(U_i)} U_i.$$

The first, second and fourth factor being similar, we will discuss only the first one. It is clear in the case of  $\Phi(X_{12}, X_{23})$  that either  $U_1$  is in  $\mathcal{W}^{12,23}$  and its coefficient is then  $Z_{\rho_1(U_1)}$ ; or  $U_1$  is not in  $\mathcal{W}^{12,23}$  and it does not appear in  $\Phi(X_{12}, X_{23})$  which means that its coefficient is 0.

The third and fifth factor are similar and thus we will treat only the former. We can write  $\Phi(X_{23} + X_{24} + X_{34}, X_{12})$  as

$$\sum_{(l, \mathbf{k}) \in \mathcal{L}_{2,c}(\mathbb{N})} Z_{X_0^{l_1} X_1^{k_1} \dots X_0^{l_p} X_1^{k_p}} (X_{23} + X_{24} + X_{34})^{l_1} X_{12}^{k_1} \dots (X_{23} + X_{24} + X_{34})^{l_p} X_{12}^{k_p}.$$

We can rewrite the previous sum as running through all the words in the letters  $X_{12}, X_{23}, X_{24}$  and  $X_{34}$  because  $(X_{23} + X_{24} + X_{34})^l$  is equal to

$$\sum_{\substack{W \in {}_{24}\mathcal{W}_{34}^{12,23} \\ |W|=l}} W.$$

Using the unique decomposition (as word) of  $U_4 \in {}_{24}\mathcal{W}_{34}^{12,23}$  as

$$U_4 = V_1 X_{12}^{k_1} \dots V_p X_{12}^{k_p} \quad \text{with } V_i \in {}_{24}\mathcal{W}_{34}^{23},$$

we see that each word  $U_4$  in  ${}_{24}\mathcal{W}_{34}^{12,23}$  appears one and only one time in  $\Phi(X_{23} + X_{24} + X_{34}, X_{12})$  with the coefficient  $Z_{X_0^{|V_1|} X_1^{k_1} \dots X_0^{|V_p|} X_1^{k_p}}$ . We finally have

$$\Phi(X_{23} + X_{24} + X_{34}, X_{12}) = \sum_{U_3 \in \mathcal{W}} Z_{\rho_3(U_3)} U_3.$$

□

Fixing a linear basis  $B$  of  $U\mathfrak{B}_5$  (1 being an element of the basis) we have for every  $W$  in  $\mathcal{W}$  a decomposition (in  $U\mathfrak{B}_5$ )

$$W = \sum_{b \in B} l_{b,W} B \quad l_{b,W} \in k$$

and then a family of relations equivalent to (III).

**Theorem 2.12.** *The relation (III) is equivalent to the family of relations*

$$\forall b \in B \ (b \neq 1) \quad \sum_{W \in \mathcal{W}} l_{b,W} C_{5,W} = 0$$

where the  $C_{5,W}$  are given by Proposition 2.11.

*Proof.* As  $B$  is a basis, for a given  $W$  in  $\mathcal{W}$  there are only finitely many  $l_{b,W}$  that are non zero. Moreover, as  $U\mathfrak{B}_5$  is a graduated vector space (the grading is given by the weight, that is the length, of the monomial) with finite dimensional graduated part, for any  $b$  in  $B$  there are only finitely many  $l_{b,W}$  that are non zero. The product  $P_5$  is equal to

$$\begin{aligned} P_5 &= \sum_{W \in \mathcal{W}} C_{5,W} W \\ &= \sum_{W \in \mathcal{W}} C_{5,W} \left( \sum_{b \in B} l_{b,W} B \right) \\ &= \sum_{b \in B} \left( \sum_{W \in \mathcal{W}} l_{b,W} C_{5,W} \right) B. \end{aligned}$$

The relation (III) tells us that

$$P_5 = 1$$

which, because 1 is in  $B$ , means that  $C_{5,\emptyset} = 1$  and

$$\forall b \in B \ (b \neq 1) \quad \sum_{W \in \mathcal{W}} l_{b,W} C_{5,W} = 0.$$

□

Using the more common basis  $B_4$  we have:

**Corollary 2.13.** *The relation (III) is equivalent to the family of relations*

$$\forall b_4 \in B_4 \ (b_4 \neq 1) \quad \sum_{W \in \mathcal{W}} l_{b_4,W} C_{5,W} = 0$$

where the  $C_{5,W}$  are given by Proposition 2.11.

*Remark 2.14.* In the case of the basis  $B_4$  one can check that the coefficients  $l_{b_4,W}$  are in  $\mathbb{Z}$ .

The previous corollary, applied to the particular case of the Drinfel'd associator and making explicit the  $C_{5,W}$  in terms of multiple zeta values, gives:

**Theorem 2.15.** *With the convention that  $\zeta^{\text{III}}(0) = 0$ , the relation (III<sub>KZ</sub>) is equivalent to the family of relations*

$$(11) \quad \forall b_4 \in B_4 \ (b_4 \neq 1) \quad \sum_W l_{b_4,W} \left( \sum_{U_1 \dots U_5 = W} (-1)^{dp_1(U_1) + dp_2(U_2) + dp_3(U_3) + dp_4(U_4) + dp_5(U_5)} \zeta^{\text{III}}(\rho_1(U_1)) \zeta^{\text{III}}(\rho_2(U_2)) \zeta^{\text{III}}(\rho_3(U_3)) \zeta^{\text{III}}(\rho_4(U_4)) \zeta^{\text{III}}(\rho_5(U_5)) \right) = 0$$

where  $dp_i(U)$  is the depth of  $\rho_i(U)$  and the words  $W, U_i$  are in  $\mathcal{W}$ .

### 3. BAR CONSTRUCTION AND ASSOCIATOR RELATIONS

In this section, we suppose that  $k$  is  $\mathbb{C}$ . We review the notion of bar construction and its links with multiple zeta values. Those results have been shown in greater generality in [Che73] and [Bro09]. We will recall the Brown variant of Chen's reduced bar construction in the case of the moduli spaces of curves of genus 0 with 4 and 5 marked points,  $\mathcal{M}_{0,4}$  and  $\mathcal{M}_{0,5}$ .

**3.1. Bar Construction.** The moduli space of curves of genus 0 with 4 marked points,  $\mathcal{M}_{0,4}$ , is

$$\mathcal{M}_{0,4} = \{(z_1, \dots, z_4) \in (\mathbb{P}^1)^4 \mid z_i \neq z_j \text{ if } i \neq j\} / \mathrm{PGL}_2(k)$$

and is identified as

$$\mathcal{M}_{0,4} \simeq \{t \in (\mathbb{P}^1) \mid t \neq 0, 1, \infty\}$$

by sending the point  $[(0, t, 1, \infty)] \in \mathcal{M}_{0,4}$  to  $t$ .

The moduli space of curves of genus 0 with 5 marked points,  $\mathcal{M}_{0,5}$ , is

$$\mathcal{M}_{0,5} = \{(z_1, \dots, z_5) \in (\mathbb{P}^1)^5 \mid z_i \neq z_j \text{ if } i \neq j\} / \mathrm{PGL}_2(k)$$

and is identified as

$$\mathcal{M}_{0,5} \simeq \{(x, y) \in (\mathbb{P}^1)^2 \mid x, y \neq 0, 1, \infty \text{ and } x \neq y\}$$

by sending the point  $[(0, xy, y, 1, \infty)] \in \mathcal{M}_{0,5}$  to  $(x, y)$ . This identification can be interpreted as the composition of

$$\mathcal{M}_{0,5} \longrightarrow \mathcal{M}_{0,4} \times \mathcal{M}_{0,4}$$

$$[(z_1, \dots, z_5)] \longmapsto [(z_1, z_2, z_3, z_5)] \times [(z_1, z_3, z_4, z_5)]$$

with the previous identification of  $\mathcal{M}_{0,4}$  using the fact that  $[(0, xy, y, \infty)] = [(0, x, 1, \infty)]$ .

For  $\mathcal{M} = \mathcal{M}_{0,4}$  or  $\mathcal{M} = \mathcal{M}_{0,5}$ , Brown has defined in [Bro09] a graded Hopf  $k$ -algebra

$$(12) \quad V(\mathcal{M}) = \bigoplus_{m=0}^{\infty} V_m(\mathcal{M}) \subset \bigoplus_{m=0}^{\infty} \mathrm{H}_{\mathrm{DR}}^1(\mathcal{M})^{\otimes m}.$$

Here  $V_0(\mathcal{M}) = k$ ,  $V_1(\mathcal{M}) = \mathrm{H}_{\mathrm{DR}}^1(\mathcal{M})$  and  $V_m(\mathcal{M})$  is the intersection of the kernel  $\wedge_i$  for  $1 \leq i \leq m-1$ :

$$\begin{aligned} \wedge_i : \mathrm{H}_{\mathrm{DR}}^1(\mathcal{M})^{\otimes m} &\longrightarrow \mathrm{H}_{\mathrm{DR}}^1(\mathcal{M})^{\otimes m-i-1} \otimes \mathrm{H}_{\mathrm{DR}}^2(\mathcal{M}) \otimes \mathrm{H}_{\mathrm{DR}}^1(\mathcal{M})^{\otimes i-1} \\ \nu_m \otimes \cdots \otimes \nu_1 &\longmapsto \nu_m \otimes \cdots \otimes (\nu_{i+1} \wedge \nu_i) \otimes \cdots \otimes \nu_1. \end{aligned}$$

Suppose that  $\omega_1, \dots, \omega_k$  form a basis of  $\mathrm{H}_{\mathrm{DR}}^1(\mathcal{M})$ , then the elements of  $V_m(\mathcal{M})$  can be written as linear combinations of symbols

$$\sum_{I=(i_1, \dots, i_m)} c_I [\omega_{i_m} | \cdots | \omega_{i_1}],$$

with  $c_I \in k$ , which satisfies the integrability condition

$$(13) \quad \sum_{I=(i_1, \dots, i_m)} c_I \omega_{i_m} \otimes \cdots \otimes \omega_{i_{j+2}} \otimes (\omega_{i_{j+1}} \wedge \omega_{i_j}) \otimes \omega_{i_{j-1}} \otimes \cdots \otimes \omega_{i_m} = 0$$

for all  $1 \leq j \leq m-1$ .

**Definition 3.1.** The Brown's bar construction over  $\mathcal{M}$  is the tensor product

$$B(\mathcal{M}) = \mathcal{O}_{\mathcal{M}} \otimes V(\mathcal{M}).$$

**Theorem 3.2** ([Bro09]). *The bar construction  $B(\mathcal{M})$  is a commutative graded Hopf algebra isomorphic to the zero<sup>th</sup> cohomology group of Chen's reduced bar complex on  $\mathcal{O}_{\mathcal{M}}$  :*

$$B(\mathcal{M}) \simeq H^0(B(\Omega^\bullet \mathcal{O}_{\mathcal{M}}))$$

Let  $\nu_m, \dots, \nu_1$  be  $m$  holomorphic 1-forms in  $\Omega^1(\mathcal{M})$  the iterate integral of the word  $\nu_m \cdots \nu_1$ ,  $\int \nu_m \circ \cdots \circ \nu_1$ , is the application that sends any path  $\gamma : [0, 1] \rightarrow \mathcal{M}$  to

$$\int_{\gamma} \nu_m \circ \cdots \circ \nu_1 = \int_{0 < t_1 < \dots < t_m} \gamma^* \nu_1(t_1) \wedge \cdots \wedge \gamma^* \nu_m(t_m),$$

The value is called the iterated integral of  $\nu_m \cdots \nu_1$  along  $\gamma$ . We extend these definitions by linearity to linear combinations of forms  $\sum_I c_I \nu_{i_m} \cdots \nu_{i_1}$ .

When the iterated integral  $\int_{\gamma} \sum_I c_I \nu_m \circ \cdots \circ \nu_1$  depends only of the homotopy class of  $\gamma$ , we say it is an homotopy invariant iterate integral and note it  $\int \sum_I c_I \nu_m \circ \cdots \circ \nu_1$ . Let  $L(\mathcal{M})$  denote the set of all the homotopy invariant iterated integral.

**Proposition 3.3** ([Bro09]). *The morphism  $\rho_{b, \gamma}$  defined as*

$$\begin{aligned} \rho : B(\mathcal{M}) &\longrightarrow L(\mathcal{M}) \\ \sum_I c_I [\omega_{i_m} | \cdots | \omega_{i_1}] &\longmapsto \int \sum_I c_I \omega_{i_m} \circ \cdots \circ \omega_{i_1} \end{aligned}$$

*is an isomorphism.*

*Remark 3.4.* In particular for any such  $\gamma$  homotopically equivalent to zero we have for all  $\sum_I c_I [\omega_{i_m} | \cdots | \omega_{i_1}]$  in  $V(\mathcal{M})$  :

$$\sum_I c_I \int_{\gamma} \omega_{i_m} \circ \cdots \circ \omega_{i_1} = 0$$

**3.2. Bar Construction on  $\mathcal{M}_{0,4}$ , symmetry and hexagon relations.** Here, we will show how the symmetry relations ( $I_{KZ}$ ) and the hexagon ( $II_{KZ}$ ) relations are related to the bar construction on  $\mathcal{M}_{0,4}$ .

First of all we should remark that  $B(\mathcal{M}_{0,4})$  is extremely simple.

**Proposition 3.5.** *Let  $\omega_0$  and  $\omega_1$  denote respectively the differential 1-form, in  $\Omega^1(\mathcal{M}_{0,4})$ ,  $\frac{dt}{t}$  and  $\frac{dt}{t-1}$ .*

*Then, any element  $[\omega_{\varepsilon_n} | \cdots | \omega_{\varepsilon_1}]$  with  $\varepsilon_i$  in  $\{0, 1\}$  is an element of  $V(\mathcal{M}_{0,4})$ . Moreover, the family of these elements is a basis of  $V(\mathcal{M}_{0,4})$ .*

Sending  $X_0$  on  $w_0$  and  $X_1$  on  $w_1$  gives a one to one correspondence between words  $W$  in  $\mathcal{W}_{0,1}$  and the elements of the previous basis of  $V(\mathcal{M}_{0,4})$  which is the dual of  $U\mathfrak{F}_2$ . By this correspondence,  $W = X_{\varepsilon_n} \cdots X_{\varepsilon_1}$  is send to its dual  $W^* = \omega_W = [\omega_{\varepsilon_n} | \cdots | \omega_{\varepsilon_1}]$

*Proof.* As  $\omega_0 \wedge \omega_1 = 0$  the integrability condition is automatically satisfied and because  $(\omega_0, \omega_1)$  the proposition follows.  $\square$

Following [Bro09] and considering the three dihedral structure on  $\mathcal{M}_{0,4}$ , one can define 6 tangential based points :  $0\vec{1}$ ,  $1\vec{0}$ ,  $1\vec{\infty}$ ,  $\infty\vec{1}$ ,  $\infty\vec{0}$  and  $0\vec{\infty}$ . Let  $p$  denote the path beginning at the tangential based point  $0\vec{1}$  and ending at  $1\vec{0}$  defined by  $t \mapsto t$  and let  $p^{-1}$  denote its inverse  $t \mapsto 1 - t$ . If  $\alpha$  and  $\beta$  are two paths in a variety with  $\alpha(1) = \beta(0)$ ,  $\beta \circ \alpha$  will be the composed path beginning with  $a$  and ending with  $b$ . Then the iterated integral of  $\omega = \omega_n \cdots \omega_1$  along  $\beta \circ \alpha$  is equal to

$$\sum_{k=0}^n \left( \int_b \omega_n \circ \cdots \circ \omega_{n-k+1} \right) \left( \int_a \omega_{n-k} \circ \cdots \circ \omega_1 \right)$$

If  $\gamma$  is a path, starting at a tangential based point  $\vec{P}$  (and/or ending at a tangential based point  $\vec{P}'$ ) an iterated integral  $\int \omega$  may be divergent. However, one can define (as in [Bro09]) a value to that divergent integral ; we speak of regularised iterated integral. If  $W$  is in  $X_0\mathcal{W}_{0,1}X_1$ , the iterated integral  $\int_p \omega_W$  is convergent and is equal to  $(-1)^{dp(W)}\zeta(W)$ . If  $W$  is in  $\mathcal{W}_{0,1} \setminus X_0\mathcal{W}_{0,1}X_1$  then the regularised iterated integral  $\int_p \omega_W$  is equal to  $(-1)^{dp(W)}\zeta^{\text{m}}(W)$ . We may, thereafter, omit the term *regularised* in the expressions “regularised iterated integral ” or “regularised homotopy invariant iterated integral”.

**Theorem 3.6.** *The relation  $(I_{KZ})$  is equivalent to the family of relation*

$$\forall W \in \mathcal{W}_{0,1} \quad \int_{p \circ p^{-1}} \omega_W = 0$$

which is exactly the family (3).

*Proof.* Considering the KZ equation (KZ)

$$\frac{\partial g}{\partial u} = \left( \frac{X_0}{u} + \frac{X_1}{1-u} \right) \cdot g(u)$$

and the two normalized solutions at 0 and 1,  $g_0$  and  $g_1$ ,  $\Phi_{KZ}(X_0, X_1)$  is the unique element in  $U\mathfrak{F}_2$  such that

$$g_0(u) = g_1(u)\Phi_{KZ}(X_0, X_1).$$

Using the symmetry of the situation we also have

$$g_1(u) = g_0(u)\Phi_{KZ}(X_1, X_0).$$

The equation  $(I_{KZ})$  comes from the unicity of such a solution normalized at 1

$$g_1(u) = g_1(u)\Phi_{KZ}(X_0, X_1)\Phi_{KZ}(X_1, X_0).$$

The elements  $\Phi_{KZ}(X_0, X_1)$  and  $\Phi_{KZ}(X_1, X_0)$  can be expressed using regularised iterated integrals as

$$\Phi_{KZ}(X_0, X_1) = \sum_{W \in \mathcal{W}_{0,1}} \left( \int_p \omega_W \right) W$$

and

$$\Phi_{KZ}(X_1, X_0) = \sum_{W \in \mathcal{W}_{0,1}} \left( \int_{p^{-1}} \omega_W \right) W.$$

The product  $\Phi_{KZ}(X_0, X_1)\Phi_{KZ}(X_1, X_0)$  is the series

$$\sum_{W \in \mathcal{W}_{0,1}} \left( \int_{p^{-1} \circ p} \omega_W \right) W.$$

As the path  $p^{-1} \circ p$  is homotopically equivalent to 0, all the previous iterated integrals are 0 and  $(I_{KZ})$  is equivalent to

$$\forall W \in \mathcal{W}_{0,1} \quad \int_{p \circ p^{-1}} \omega_W = 0.$$

Lets, now, fix any  $W = X_{\varepsilon_n} \cdots X_{\varepsilon_1}$  in  $\mathcal{W}_{0,1}$  and compute the regularised iterated integral  $\int_{p \circ p^{-1}} \omega_W = 0$ . We have

$$\int_{p \circ p^{-1}} \omega_W = \sum_{k=0}^n \left( \int_p \omega_{\varepsilon_n} \circ \cdots \circ \omega_{\varepsilon_{n-k+1}} \right) \left( \int_{p^{-1}} \omega_{\varepsilon_{n-k}} \circ \cdots \circ \omega_{\varepsilon_1} \right).$$

Setting  $U_1 = X_{\varepsilon_n} \cdots X_{\varepsilon_{n-k+1}}$  and  $U_2 = X_{\varepsilon_{n-k}} \cdots X_{\varepsilon_1}$ , we have

$$\int_p \omega_{\varepsilon_n} \circ \cdots \circ \omega_{\varepsilon_{n-k+1}} = (-1)^{dp(U_1)}\zeta^{\text{m}}(U_1).$$



As  $p^{-1}$  is given by  $t \mapsto 1 - t$  we have  $(p^{-1})^*(\omega_\varepsilon) = \omega_{1-\varepsilon}$  for  $\varepsilon = 0, 1$  and because  $p^*(\omega_\varepsilon) = \omega_\varepsilon$  we have

$$\begin{aligned} \int_{p^{-1}} \omega_{\varepsilon_{n-k}} \circ \cdots \circ \omega_{\varepsilon_1} &= \int_{0 < t_1 < \cdots < t_{n-k}} (p^{-1})^*(\omega_{\varepsilon_1}(t_1) \wedge \cdots \wedge (p^{-1})^*(\omega_{\varepsilon_{n-k}}(t_{n-k})) \\ &= \int_{0 < t_1 < \cdots < t_{n-k}} (\omega_{1-\varepsilon_1}(t_1) \wedge \cdots \wedge (\omega_{1-\varepsilon_{n-k}}(t_{n-k})) \\ &= \int_p \omega_{1-\varepsilon_{n-k}} \circ \cdots \circ \omega_{1-\varepsilon_1} = \int_p \omega_{\theta(U_2)}, \end{aligned}$$

where  $\theta$  exchange  $X_0$  and  $X_1$ . Finally we have

$$\int_{p^{-1}} \omega_{U_2} = \int_p \omega_{\theta(U_2)} = (-1)^{dp(\theta(U_2))} \zeta^{\text{III}}(U_2)$$

and

$$0 = \int_{p \circ p^{-1}} \omega_W \sum_{U_1 U_2 = W} (-1)^{dp(U_1)} \zeta^{\text{III}}(U_1) (-1)^{dp(\theta(U_2))} \zeta^{\text{III}}(U_2)$$

which is exactly the relation (3) for the word  $W$ .  $\square$

Now, let  $c$  be the infinitesimal half circle around 0 in the lower half plan, connecting the tangential based point  $0\vec{\infty}$  and  $0\vec{1}$ . The path  $c$  can be seen as the limit when  $\varepsilon$  tends to 0 of  $c_\varepsilon : t \mapsto \varepsilon e^{i(\pi+t\pi)}$ . We have a natural 3 cycle on  $\mathcal{M}_{0,4}$  given by  $\tau : t \mapsto \frac{1}{1-t}$  and let  $\gamma$  be the path  $c \circ \tau^2(p) \circ \tau^2(c) \circ \tau(p) \circ \tau(c) \circ p$ .

**Theorem 3.7.** *The relation  $(\text{II}_{\text{KZ}})$  is equivalent to the family of relation*

$$\forall W \in \mathcal{W}_{0,1} \quad \int_\gamma \omega_W = 0$$

which is exactly the family (8).

*Proof.* Comparing the six different normalized solutions of (KZ) at the six different based points leads to  $(\text{II}_{\text{KZ}})$  via the relation

$$g_0(u) = g_0(u) e^{i\pi X_0} \Phi_{\text{KZ}}(X_\infty, X_0) e^{i\pi X_\infty} \Phi_{\text{KZ}}(X_1, X_\infty) e^{i\pi X_1} \Phi_{\text{KZ}}(X_0, X_1)$$

where the exponentials are coming from the monodromy around 0, 1 and  $\infty$ . The product in  $U\mathfrak{F}_2$  in the R.H.S of the previous equation can be expressed using homotopy invariant iterated integrals

$$e^{i\pi X_0} \Phi_{\text{KZ}}(X_\infty, X_0) e^{i\pi X_\infty} \Phi_{\text{KZ}}(X_1, X_\infty) e^{i\pi X_1} \Phi_{\text{KZ}}(X_0, X_1) = \sum_{W \in \mathcal{W}_{0,1}} \left( \int_\gamma \omega_W \right) W$$

because one compare the different solutions using analytic continuation along paths. So the comparison of the six different solutions correspond exactly to an analytic continuation along any path starting at  $0\vec{1}$ , joining the other tangential based points  $1\vec{0}$ ,  $1\vec{\infty}$ ,  $\infty\vec{1}$ ,  $\infty\vec{0}$ ,  $0\vec{\infty}$  in that order and ending at  $0\vec{1}$ ; staying all the time in the lower half plan.

As  $\gamma$  is homotopically equivalent to 0, the first part of theorem follows because for any word  $W$  in  $\mathcal{W}_{0,1}$ ,  $\omega_W$  give rise to an homotopy invariant iterated integral.

Using the decomposition of iterated integral on a composed path we have

$$\begin{aligned} \forall W \in \mathcal{W}_{0,1} \quad \int_\gamma \omega_W &= \sum_{\substack{U_1, \dots, U_6 \\ U_1 \cdots U_6 = W}} \int_c \omega_{U_1} \int_{\tau^2(p)} \omega_{U_2} \int_{\tau^2(c)} \omega_{U_3} \\ &\quad \int_{\tau(p)} \omega_{U_4} \int_{\tau(c)} \omega_{U_5} \int_p \omega_{U_6}. \end{aligned}$$

Thus, in order to show that it gives exactly the family of relations (8), it is enough, to show that for any  $U$  in  $\mathcal{W}_{0,1}$

$$\begin{aligned} \int_c \omega_U &= C_{0,1}(e^{i\pi X_0}|U), & \int_{\tau^2(p)} \omega_U &= C_{0,1}(\Phi_{KZ}(X_\infty, X_0)|U), \\ \int_{\tau^2(c)} \omega_U &= C_{0,1}(e^{i\pi X_\infty}|U), & \int_{\tau(p)} \omega_U &= C_{0,1}(\Phi_{KZ}(X_1, X_\infty)|U), \\ \int_{\tau(c)} \omega_U &= C_{0,1}(e^{i\pi X_1}|U), & \int_p \omega_U &= C_{0,1}(\Phi_{KZ}(X_0, X_1)|U). \end{aligned}$$

In order to compute the iterated integral along  $c$ ,  $\tau(c)$  and  $\tau^2(c)$ , it is enough to compute the limit when  $\varepsilon$  tends to 0 of the iterate integral along  $c_\varepsilon$ ,  $\tau(c_\varepsilon)$  and  $\tau^2(c_\varepsilon)$ . As

$$c_\varepsilon^*(\omega_0) = i\pi dt \quad \text{and} \quad c_\varepsilon^*(\omega_1) = \varepsilon \frac{-i\pi e^{i(\pi+\pi t)} dt}{1 - \varepsilon e^{i(\pi+\pi t)}},$$

the iterate integral  $\int_{c_\varepsilon} \omega_U$  tends to 0 except if  $U = X_0^n$  and then  $\int_{c_\varepsilon} \omega_{X_0^n} = \frac{(i\pi)^n}{n!}$  for all  $\varepsilon$ . Thus, we have

$$\int_c \omega_U = C_{0,1}(e^{i\pi X_0}|U).$$

Similarly we have

$$\tau(c_\varepsilon)^*(\omega_1) = i\pi \frac{dt}{1 - \varepsilon e^{i(\pi+\pi t)}} \quad \text{and} \quad \tau(c_\varepsilon)^*(\omega_0) = \frac{\varepsilon i\pi e^{i(\pi+\pi t)} dt}{1 - \varepsilon e^{i(\pi+\pi t)}}$$

and the iterate integral  $\int_{\tau(c_\varepsilon)} \omega_U$  tends to 0 except if  $U = X_1^n$  and then  $\int_{c_\varepsilon} \omega_{X_0^n}$  tends to  $\frac{(i\pi)^n}{n!}$  when  $\varepsilon$  tends to 0. Thus, we have

$$\int_{\tau(c)} \omega_U = C_{0,1}(e^{i\pi X_1}|U).$$

Computing  $\tau^2(c_\varepsilon)^*$ , we have

$$\tau^2(c_\varepsilon)^*(\omega_0) = -i\pi \frac{dt}{1 - \varepsilon e^{i(\pi+\pi t)}} \quad \text{and} \quad \tau^2(c_\varepsilon)^*(\omega_1) = -i\pi dt$$

and we find that the limit when  $\varepsilon$  tends to 0 of  $\int_{\tau^2(c_\varepsilon)} \omega_U$  is  $\frac{(-i\pi)^{|U|}}{|U|!}$  which gives

$$\int_{\tau^2(c)} \omega_U = C_{0,1}(e^{i\pi X_\infty}|U).$$

The equality  $\int_p \omega_U = C_{0,1}(\Phi_{KZ}(X_0, X_1)|U)$  is obvious and the case of  $\int_{\tau(p)} \omega_U$  and  $\int_{\tau^2(p)} \omega_U$  are extremely similar so we will discuss only the last one. First, we should remark that

$$\tau^2(c)^*(\omega_0) = -\omega_0 + \omega_1 \quad \text{and} \quad \tau^2(c)^*(\omega_1) = -\omega_0.$$

As, for  $U = X_{\varepsilon_n} \cdots X_{\varepsilon_1}$  ( $\varepsilon_i = 0, 1$ ) we can rewrite the iterate integral  $\int_{\tau^2(c)} \omega_U$  as

$$\int_p \tau^2(p)^*(\omega_{\varepsilon_n}) \circ \cdots \circ \tau^2(p)^*(\omega_{\varepsilon_1}).$$

We will now prove by induction on  $n = |U|$  that in  $V(\mathcal{M}_{0,4})$

$$(14) \quad [\tau^2(p)^*(\omega_{\varepsilon_n}) | \cdots | \tau^2(p)^*(\omega_{\varepsilon_1})] = \sum_{(\mathbf{V}, \mathbf{k}) \in \text{deco}_{0,1}(U, X_0)} (-1)^{|\mathbf{V}|} \omega_{X_0^{|\mathbf{V}_1|} X_1^{k_1} X_0^{|\mathbf{V}_2|} X_1^{k_2} \cdots X_0^{|\mathbf{V}_p|} X_1^{k_p}}$$

which will give using Proposition 2.7 the equality

$$\int_p \omega_U = C_{0,1}(\Phi_{KZ}(X_0, X_1)|U).$$

If  $U = X_0$ ,  $\text{dec}_{0,1}(U, X_0)$  have 2 elements,  $((X_0), (0))$  and  $((\emptyset), (1))$ ; if  $U = X_1$  then  $\text{dec}_{0,1}(U, X_0)$  have only one element  $((X_1), (0))$ . In both cases (14) is satisfied.

For the simplicity of notation, if  $W = X_{j_n} \cdots X_{j_1}$  ( $j_i = 0, 1$ ) is in  $\mathcal{W}_{0,1}$ , we shall write  $[\omega_W|\omega_\varepsilon]$  for  $[\omega_{j_n}|\cdots|\omega_{j_1}|\omega_\varepsilon]$ . We suppose now that  $U = U_1 X_0$  with  $|U_1| \geq 1$ . We have a map from  $\text{dec}_{0,1}(U, X_0)$  to  $\text{dec}_{0,1}(U_1, X_0)$  that sends a decomposition  $(\mathbf{V}, \mathbf{k})$  with  $\mathbf{V} = (V_1, \dots, V_p)$  and  $\mathbf{k} = (k_1, \dots, k_p)$  to

$$\begin{cases} (\mathbf{V}, (k_1, \dots, k_p - 1)) & \text{if } k_r \neq 0 \\ ((V_1, \dots, V_p'), \mathbf{k}) & \text{if } k_p = 0 \text{ and } V_p = V_p' X_0. \end{cases}$$

Any decomposition  $(\mathbf{V}', \mathbf{k}')$  in  $\text{dec}_{0,1}(U_1, X_0)$  has exactly two preimages by this map. If one write  $U_1' = V_1' X_0^{k_1'} \cdots V_p' X_0^{k_p'}$  then it leads to two decompositions of  $U$

$$((V_1', \dots, V_p'), (k_1', \dots, k_p' + 1)) \quad \text{and} \quad ((V_1', \dots, V_p', X_0), (k_1', \dots, k_p', 0)).$$

By induction we have in  $V_{n-1}(\mathcal{M}_{0,4})$

$$[\tau^2(p)^*(\omega_{\varepsilon_n})|\cdots|\tau^2(p)^*(\omega_{\varepsilon_2})] = \sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \text{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|} \omega_{X_0^{|\mathbf{V}'|} X_1^{k_1'} \cdots X_0^{|\mathbf{V}'|} X_1^{k_p'}}.$$

We deduce from the previous equality and using the linearity of the tensor product that  $[\tau^2(p)^*(\omega_{\varepsilon_n})|\cdots|\tau^2(p)^*(\omega_{\varepsilon_1})]$  is equal to

$$\sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \text{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|} [\omega_{X_0^{|\mathbf{V}'|} X_1^{k_1'} \cdots X_0^{|\mathbf{V}'|} X_1^{k_p'}} | -\omega_0 + \omega_1],$$

which can be decomposed as

$$\begin{aligned} \sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \text{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|+1} [\omega_{X_0^{|\mathbf{V}'|} X_1^{k_1'} \cdots X_0^{|\mathbf{V}'|} X_1^{k_p'}} |\omega_0] + \\ \sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \text{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|} [\omega_{X_0^{|\mathbf{V}'|} X_1^{k_1'} \cdots X_0^{|\mathbf{V}'|} X_1^{k_p'}} |\omega_1]. \end{aligned}$$

The first term of the sum is equal to  $\sum_{(\mathbf{V}', \mathbf{k}')} (-1)^{|\mathbf{V}'|+1} \omega_{X_0^{|\mathbf{V}'|} X_1^{k_1'} \cdots X_0^{|\mathbf{V}'|} X_1^{k_p'} X_0}$  and the second term is equal to  $\sum_{(\mathbf{V}', \mathbf{k}')} (-1)^{|\mathbf{V}'|} \omega_{X_0^{|\mathbf{V}'|} X_1^{k_1'} \cdots X_0^{|\mathbf{V}'|} X_1^{k_p'+1}}$ . This gives (14) when  $U = U_1' X_0$ .

If  $U = U_1 X_1$  with  $|U_1| \geq 1$ , we have a one to one correspondence between  $\text{dec}_{0,1}(U_1, X_0)$  and  $\text{dec}_{0,1}(U, X_0)$  defined by

$$((V_1', \dots, V_p'), (k_1', \dots, k_p')) \mapsto \begin{cases} ((V_1', \dots, V_p', X_1), (k_1', \dots, k_p', 0)) & \text{if } k_p' = 0 \\ ((V_1', \dots, V_p', X_1), (k_1', \dots, k_p')) & \text{otherwise.} \end{cases}$$

Then, (14) follows by induction using the linearity of the tensor product.  $\square$

**3.3. Bar Construction on  $\mathcal{M}_{0,5}$  and the pentagon relations.** Here, we will show how the pentagon relations ( $\Pi_{KZ}$ ) are related to the bar construction on  $\mathcal{M}_{0,5}$ .

The shuffle algebra  $B(\mathcal{M}_{0,4})$  being much more complicated than  $B(\mathcal{M}_{0,4})$  we will first review some facts explained in [Bro09]. We now fix a dihedral structure  $\delta$ , as described in [Bro09], on  $\mathcal{M}_{0,5}$  given by  $z_1 < z_2 < z_3 < z_4 < z_5$ , or with our normalization  $0 < xy < y < 1 < \infty$ . This corresponds to choosing the good coordinates to study the connected component of  $\mathcal{M}_{0,5}(\mathbb{R})$  such that the marked

points are in the order given by  $\delta$ . We will refer to that component as the standard cell. Let  $\omega_{12}, \omega_{23}, \omega_{34}, \omega_{45}, \omega_{24}$  be respectively the differential forms  $d \log(u_{25}) = \frac{dx}{x}$ ,  $d \log(u_{31}u_{41}) = \frac{dx}{x-1}$ ,  $d \log(u_{24}u_{41}) = \frac{dy}{y-1}$ ,  $d \log(u_{35}) = \frac{dy}{y}$  and  $d \log(u_{41}) = \frac{d(xy)}{xy-1}$ .

If  $W$  is a word in  $\mathcal{W} = \{X_{34}, X_{45}, X_{24}, X_{12}, X_{23}\}^*$  with  $|W| = n$ , we will write  $\omega_W \in \mathbb{H}_{\text{DR}}(\mathcal{M}_{0,5})^{\otimes n}$  the bar symbol  $[\omega_{i_n j_n} | \cdots | \omega_{i_1 j_1}]$ . Note that the elements  $\omega_W$  for  $W$  in  $\mathcal{W}$  are not all in  $V(\mathcal{M}_{0,5})$  usually, only linear combination of such symbols are in  $V(\mathcal{M}_{0,5})$ .

**Example 3.8.** The elements  $[\omega_{12}]$ ,  $[\omega_{23}]$  and  $[\omega_{12}|\omega_{23}]$  are in  $V(\mathcal{M}_{0,5})$  even if  $[\omega_{12}|\omega_{45}]$  is not. However  $[\omega_{12}|\omega_{45}] + [\omega_{45}|\omega_{12}]$  is in  $V(\mathcal{M}_{0,5})$ .

Example 3.43 (via the Theorem 3.38 and Corollary 3.41) in [Bro09] tells us that the exact sequence

$$0 \longrightarrow \mathbb{C}\langle\langle X_{24}, X_{34}, X_{45} \rangle\rangle \longrightarrow U\mathfrak{B}_5 \longrightarrow \mathbb{C}\langle\langle X_{12}, X_{23} \rangle\rangle \longrightarrow 0$$

is dual to

$$0 \longrightarrow V(\mathcal{M}_{0,4}) \longrightarrow V(\mathcal{M}_{0,5}) \longrightarrow \mathbb{C}\left\langle \frac{dy}{y}, \frac{dy}{y-1}, \frac{x dy}{xy-1} \right\rangle \longrightarrow 0$$

which comes from the expression in cubical coordinates of  $\mathcal{M}_{0,5} \longrightarrow \mathcal{M}_{0,4}$  forgetting the 4th point. Thus the identification

$$U\mathfrak{B}_5 \simeq \mathbb{C}\langle\langle X_{24}, X_{34}, X_{45} \rangle\rangle \rtimes \mathbb{C}\langle\langle X_{12}, X_{23} \rangle\rangle$$

is dual to

$$V(\mathcal{M}_{0,5}) \simeq V(\mathcal{M}_{0,4}) \otimes \mathbb{C}\left\langle \frac{dy}{y}, \frac{dy}{y-1}, \frac{x dy}{xy-1} \right\rangle$$

and  $V(\mathcal{M}_{0,5})$  is the dual of  $U\mathfrak{B}_5$ .

The graded dual of the free algebra of formal series

$$R = k\langle\langle X_{34}, X_{45}, X_{24}, X_{12}, X_{23} \rangle\rangle$$

is the shuffle algebra

$$T := \bigoplus_n (k\omega_{34} \oplus k\omega_{45} \oplus k\omega_{24} \oplus k\omega_{12} \oplus k\omega_{23})^{\otimes n}.$$

Let  $\Omega$  be the element in  $R \otimes \mathbb{H}_{\text{DR}}^1(\mathcal{M}_{0,5})$  defined by

$$\Omega = X_{12} \otimes \omega_{12} + X_{23} \otimes \omega_{23} + X_{34} \otimes \omega_{34} + X_{45} \otimes \omega_{45} + X_{24} \otimes \omega_{24}.$$

and

$$\text{Exp}(\Omega) := \sum_{W \in \mathcal{W}} W \otimes \omega_W \in R \otimes T.$$

The element  $\text{Exp}(\Omega)$  corresponds to the identity of  $R$  and encodes the fact that the dual of a word  $W$  is  $\omega_W$ . Using the projection  $R \rightarrow U\mathfrak{B}_5$  one can see  $\text{Exp}(\Omega)$  in  $U\mathfrak{B}_5 \otimes T$ . A word  $W$  (seen in  $U\mathfrak{B}_5$ ) is written in the basis  $B_4$  as

$$W = \sum_{b_4 \in B_4} l_{b_4, W} b_4.$$

Duality between  $R$  and  $T$  and between  $U\mathfrak{B}_5$  and  $V(\mathcal{M}_{0,5})$  tells us that the dual basis  $B_4^* = (b_4^*)$  of  $B_4$  is given by

$$\forall b_4 \in B_4 \quad b_4^* = \sum_{W \in \mathcal{W}} l_{b_4, W} \omega_W.$$

So, writing each  $W$  in the expression  $\text{Exp}(\Omega)$  in the basis  $B_4$  leads to

$$\text{Exp}(\Omega) = \sum_{b_4 \in B_4} b_4 \otimes b_4^* \in U\mathfrak{B}_5^* \simeq V(\mathcal{M}_{0,5})$$

and  $\text{Exp}(\Omega)$  realized the identification between the graded dual of  $U\mathfrak{B}_5$  and  $V(\mathcal{M}_{0,5})$  as it was remarked by Furusho in [Fur08]. This discussion can be resumed by the following proposition.

**Proposition 3.9.** *We have a natural identification*

$$U\mathfrak{B}_5^* \simeq V(\mathcal{M}_{0,5})$$

where  $U\mathfrak{B}_5^*$  is the graded dual of  $U\mathfrak{B}_5$ .

This identification gives us a basis  $B_4^*$  of  $V(\mathcal{M}_{0,5})$  dual to the basis  $B_4$  of  $U\mathfrak{B}_5$  which comes from the identification

$$U\mathfrak{B}_5 \simeq k\langle\langle X_{24}, X_{34}, X_{45} \rangle\rangle \rtimes k\langle\langle X_{12}, X_{23} \rangle\rangle$$

and is explicitly given for all  $b_4$  in the basis  $B_4$  by

$$b_4^* = \sum_{W \in \mathcal{W}} l_{b_4, W} \omega_W.$$

Let  $\widehat{\mathcal{M}}_{0,5}$  be the universal covering of  $\mathcal{M}_{0,5}$ . A multi-valued function on  $\mathcal{M}_{0,5}$  is an analytic function on  $\widehat{\mathcal{M}}_{0,5}$ . Consider the formal differential equation on  $\widehat{\mathcal{M}}_{0,5}$

$$dL = \Omega L$$

where  $L$  takes values in  $U\mathfrak{B}_5$ , its coefficients being multi-valued functions on  $\mathcal{M}_{0,5}$ . As in the case of the equation (KZ), if we fix the value of  $L$  at some point of  $\mathcal{M}_{0,5}$  or its asymptotic behavior at a tangential based points, the solution is unique.

The irreducible components of  $\mathcal{M}_{0,5}$  are in one to one correspondence with the 2-partitions of  $\{z_1, z_2, z_3, z_4, z_5\}$  and will be denoted as  $z_{i_1} z_{i_2} | z_{i_3} z_{i_4} z_{i_5}$ . We will here only consider the following components  $D_{52} = z_1 z_2 | z_3 z_4 z_5$ ,  $D_{13} = z_2 z_3 | z_4 z_5 z_1$ ,  $D_{24} = z_3 z_4 | z_5 z_1 z_2$ ,  $D_{35} = z_4 z_5 | z_1 z_2 z_3$ ,  $D_{41} = z_5 z_1 | z_2 z_3 z_4$  (we may use the convention  $D_{ij} = D_{ji}$ ). Remarks that those components are given by a partition that respect the dihedral structure  $\delta$  and the numbering  $D_{ij}$  is coherent with the notation of [Bro09]. The divisors  $D_{ij}$  are given in the dihedral coordinates by  $u_{ij} = 0$ . Following Brown, we have 5 tangential based points (corresponding to the intersection of 2 irreducible components) given by the triangulation of the polygon corresponding to  $\delta$ ; as we are working in  $\mathcal{M}_{0,5}$  the polygon is a pentagon and a triangulation is given by two chords going out from a single vertex so one can number the triangulation by the number of its vertex, precisely one have

$$\begin{aligned} P_3 &= D_{35} \cap D_{13}, & P_1 &= D_{13} \cap D_{41}, & P_4 &= D_{41} \cap D_{24}, & \text{and} \\ P_2 &= D_{24} \cap D_{52}, & P_5 &= D_{52} \cap D_{35}. \end{aligned}$$

Let  $L_i$  be the normalized solution at  $P_i$  (see [Bro09] Theorem 6.12). The description of the situation in dimension 1 and section 5.2 in [Bro09] show that Theorem 6.27 of the Brown's paper that can be rewritten as

**Proposition 3.10.** *For any tangential based point and any basis  $B$  of  $U\mathfrak{B}_5$ ,  $P_i$  one can write  $L_i(z)$  as*

$$L_i(z) = \sum_{b \in B} \left( \int_{\gamma} b^* \right) b$$

where  $\gamma$  is (up to homotopy) a path from  $P_i$  to  $z$ ,  $b^*$  is the dual element in  $V(\mathcal{M}_{0,5})$  to  $b$  and where the iterated integral is a regularised iterated integral.

Comparison of two different normalized solutions at two different based points  $P_i$  and  $P_j$  is then given by

$$\forall z \in \widehat{\mathcal{M}}_{0,5} \quad L_i(z) = L_j(z) \left( \sum_{b \in B} \left( \int_{\gamma} b^* \right) b \right)$$

where  $\gamma$  is any path going from  $P_i$  to  $P_j$  homotopically equivalent to a path  $\gamma'$  going from  $P_i$  to  $P_j$  in the standard cell of  $\mathcal{M}_{0,5}(\mathbb{R})$ .

Brown shows how to restrict any element  $\omega$  in  $B(\mathcal{M}_{0,5})$  to any boundary components  $D$  introducing a regularisation map  $\text{Reg}(\omega, D)$  that send each  $\frac{du_{ij}}{u_{ij}}$  to 0 if  $u_{ij} = 0$  or if  $u_{ij} = 1$  on  $D$ .

**Proposition 3.11.** *For any two consecutive tangential based points  $P_i$  and  $P_j$  with  $j \cong i - 2 \pmod{5}$ , one have*

$$\forall z \in \widehat{\mathcal{M}}_{0,5} \quad L_i(z) = L_j(z) \left( \sum_{b \in B} \left( \int_{p_{ji}} \text{Reg}(b^*, D_{ji}) \right) b \right)$$

Where  $p_{ji}$  is the real segment going in  $D_{ji}$  from  $P_i$  to  $P_j$ .

*Proof.* The symmetry of the situation allows us to prove it only in the case where  $i = 5, j = 3$  and  $B$  is the basis  $B_4$ . Let  $p_{35}$  be the path in  $D_{35}$  going from  $P_5$  to  $P_3$ , we need to show that

$$L_5(z)^{-1} L_3(z) = Z^{53} = \sum_{b_4 \in B_4} \left( \int_{p_{35}} \text{Reg}(b_4^*, D_{35}) \right) b.$$

Using the proof of Theorem 6.20, we have

$$L_3(z)^{-1} L_5(z) = Z^{35} = \sum_{\substack{\bar{W} = [X_{i_n, j_n} | \dots | X_{i_1, j_1}] \\ \in \{X_{12}, X_{23}\}}} \left( \int_p \frac{dt}{t - \varepsilon_n} \wedge \dots \wedge \frac{dt}{t - \varepsilon_1} \right) W$$

with  $\varepsilon_k = 0$  if  $i_k = 1$  (and  $j_k = 2$ ) and  $\varepsilon_k = 1$  otherwise.

As

$$\text{Reg}(u_{25}, D_{35}) = t, \quad \text{Reg}(u_{31}, D_{35}) = 1 - t$$

$\text{Reg}(\omega_{ij}, D_{35}) = 0$  or 1 otherwise. Thus, we have

$$\text{Reg}(\omega_{12}, D_{35}) = \frac{dt}{t} \quad \text{and} \quad \text{Reg}(\omega_{23}, D_{35}) = \frac{dt}{t-1}$$

and  $\text{Reg}(u_{ij}, D_{35}) = 0$  otherwise. We need to show that if  $b_4 \in B_4$  and  $b_4$  is a word in  $\{X_{12}, X_{23}\}$  then

$$b_4^* = (X_{i_n, j_n} \dots X_{i_1, j_1})^* = [\omega_{i_n, j_n} | \dots | \omega_{i_1, j_1}]$$

and we need to show that if  $b_4$  contains some  $X_{ij}$  with  $i = 4$  or  $j = 4$  then  $b_4^*$  is a linear combination of  $\omega_W$  with  $W$  containing at least one of the letters  $X_{34}, X_{45}, X_{24}$ . Using the description of  $b_4^*$ , it follows directly from the relation defining  $U\mathfrak{B}_5$  and the proposition is proved.  $\square$

From the previous proposition we have immediately that

**Corollary 3.12.** *For any path  $\gamma$  in the standard cell homotopically equivalent to  $p_{ji}$   $j = i - 2 \pmod{5}$  we have*

$$\forall \omega \in V(\mathcal{M}_{0,5}) \quad \int_{\gamma} \omega = \int_{p_{ji}} \text{Reg}(\omega, D_{ji})$$

Let  $\gamma = p_{35} \circ p_{52} \circ p_{24} \circ p_{41} \circ p_{13}$  denotes the composed path beginning and ending at  $P_3$  and extending the map  $\text{Reg}(\omega, \gamma)$  to paths that are piecewise in some on the divisor  $D_{ij}$

**Theorem 3.13.** *The relation (III<sub>KZ</sub>) is equivalent to the family of relations*

$$\forall b_4 \in B_4 \quad \int_{\gamma} \text{Reg}(b_4^*, \gamma) = 0$$

which is exactly the family (11).

*Proof.* Comparison between the normalized solution at  $P_3$  and at  $P_3$  going through the normalized solution at  $P_1, P_4, P_2$  and  $P_5$  one find that

$$\forall z \in \widehat{\mathcal{M}}_{0,5} \quad L_3(z) = L_3(z)Z^{53}Z^{25}Z^{42}Z^{14}Z^{31}.$$

In one hand the product of the  $Z^{ij}$  is equal to 1 which is equation (III<sub>KZ</sub>) as it is shown in the proof of Theorem 6.20 [Bro09] and in the example which follows. In the other hand, the product of the  $Z^{ij}$  is given by analytic continuation along any path  $\gamma'$  in the standard cell going trough the tangential based points  $P_i$ .

$$Z^{53}Z^{25}Z^{42}Z^{14}Z^{31} = \sum_{b_4 \in B_4} \left( \int_{\gamma'} b_4^* \right) b_4.$$

Any such path being homotopically equivalent to  $\gamma$  we have

$$\int_{\gamma'} b_4^* = \int_{\gamma} \text{Reg}(b_4^*, \gamma).$$

As  $\gamma$  (and any previous  $\gamma'$ ) are homotopically equivalent to 0 each of the homotopy invariant regularised iterated integrals above are 0 (except for  $b_4 = 1$ ) which gives that the product of the  $Z^{ij}$  is equal to 1 and so relation (III<sub>KZ</sub>).

Using the expression of  $b_4^*$  in terms of  $\omega_W$ , the end of the theorem follows from Proposition 3.15.  $\square$

An immediate corollary is

**Corollary 3.14.** *For any basis  $B$  of  $U\mathfrak{B}_5$ , the pentagon relation (III<sub>KZ</sub>) is equivalent to*

$$\forall b \in B \quad \int_{\gamma} \text{Reg}(b^*, \gamma) = 0$$

where  $\gamma$ , as previously, is the path  $= p_{35} \circ p_{52} \circ p_{24} \circ p_{41} \circ p_{13}$ .

Following the proof of 3.11 one can check that

**Proposition 3.15.** *For all bar symbol  $\omega_W$  dual to a word  $W$  in the letters  $X_{34}, X_{45}, X_{24}, X_{12}, X_{23}$ , we have*

$$C_{5,W} = \int_{\gamma} \text{Reg}(\omega_W, \gamma)$$

where  $C_{5,W}$  is the coefficient defined in (9) in the case of the Drinfel'd associator  $\Phi_{KZ}$ .

*Proof.* To show the proposition, it is enough, using the decomposition of  $\gamma = p_{35} \circ p_{52} \circ p_{24} \circ p_{41} \circ p_{13}$ , to show that, for any  $U$  in  $\{X_{34}, X_{45}, X_{24}, X_{12}, X_{23}\}^*$  and any  $i$ , one have

$$Z^{\rho_i(U)} = \int_{I_i} \text{Reg}(\omega_W, I_i)$$

where  $I_5 = p_{13}$ ,  $I_4 = p_{41}$ ,  $I_3 = p_{24}$ ,  $I_2 = p_{52}$  and  $I_1 = p_{35}$ . As we have that  $\text{Reg}(\omega_{kl}, I_i) = \omega_{\rho_i(X_{kl})}$ , the corollary follows.  $\square$

#### 4. APPENDIX

Here one can find the explicit relation given by the pentagon equation III<sub>KZ</sub> in low degree. Writing the product

$$\begin{aligned} \Phi_{KZ}(X_{12}, X_{23})\Phi_{KZ}(X_{34}, X_{45})\Phi_{KZ}(X_{51}, X_{12})\Phi_{KZ}(X_{23}, X_{34}) \\ \Phi_{KZ}(X_{45}, X_{51}) = \sum_{b_4} C_{b_4} b_4 \end{aligned}$$

in the basis  $B_4$  the following tables give the relation  $C_{b_4} = 0$  in terms of regularised multiple zeta values.

4.1. **Degree 1, 2 and 3.** In degree 1 the basis is given by the letters  $X_{34}$ ,  $X_{45}$ ,  $X_{24}$ ,  $X_{12}$  and  $X_{23}$ . The relation (III<sub>KZ</sub>) in degree 1 gives.

Monomial	Dual bar symbol	Relations
$X_{1,2}$	$[\omega_{1,2}]$	$\zeta^{\text{III}}(X_0) - \zeta^{\text{III}}(X_1) = 0$
$X_{2,3}$	$[\omega_{2,3}]$	$2(\zeta^{\text{III}}(X_0) - \zeta^{\text{III}}(X_1)) = 0$
$X_{2,4}$	$[\omega_{2,4}]$	$\zeta^{\text{III}}(X_0) - \zeta^{\text{III}}(X_1) = 0$
$X_{3,4}$	$[\omega_{3,4}]$	$2(\zeta^{\text{III}}(X_0) - \zeta^{\text{III}}(X_1)) = 0$
$X_{4,5}$	$[\omega_{4,5}]$	$\zeta^{\text{III}}(X_0) - \zeta^{\text{III}}(X_1) = 0$

TABLE 1. Explicit set of relation equivalent to III<sub>KZ</sub> in degree 1

In degree 2 the basis  $B_4$  is given by 19 monomials but we have only 4 multiplicative generators and the corresponding relations are given in Table 4.1 ; in degree 3 there are 10 multiplicative generators and the corresponding relations are given in Table 4.1. There, we have write in bold the particular monomial whose dual are multiplicative generator of  $V(\mathbb{M}_{0,5})$ .

In degree 4 and 5 the family of relation equivalent to III<sub>KZ</sub> can be found on the web page of the author together with the sources of the Mathematica code.

Monomial	Dual bar symbol	Relations
$X_{2,4}X_{4,5}$	$-[\omega_{1,2} \omega_{2,4}] + [\omega_{2,4} \omega_{4,5}]$	$\zeta^{\text{III}}(X_0)\zeta^{\text{III}}(X_1) - \zeta^{\text{III}}(X_1)^2 = 0$
$X_{2,4}X_{3,4}$	$-[\omega_{1,2} \omega_{2,4}] + [\omega_{2,3} \omega_{2,4}] - [\omega_{2,3} \omega_{3,4}] + [\omega_{2,4} \omega_{3,4}]$	$-\zeta^{\text{III}}(X_0)^2 + \zeta^{\text{III}}(X_1)\zeta^{\text{III}}(X_0) - 2\zeta^{\text{III}}(X_1)^2 + \zeta^{\text{III}}(X_0X_0) + \zeta^{\text{III}}(X_0X_1) + \zeta^{\text{III}}(X_1X_0) + \zeta^{\text{III}}(X_1X_1) = 0$
$X_{3,4}X_{4,5}$	$[\omega_{3,4} \omega_{4,5}]$	$2\zeta^{\text{III}}(X_0)^2 - \zeta^{\text{III}}(X_1)\zeta^{\text{III}}(X_0) - \zeta^{\text{III}}(X_0X_1) - \zeta^{\text{III}}(X_1X_0) = 0$
$X_{1,2}X_{2,3}$	$[\omega_{1,2} \omega_{2,3}]$	$2\zeta^{\text{III}}(X_0)^2 - 2\zeta^{\text{III}}(X_1)\zeta^{\text{III}}(X_0) + \zeta^{\text{III}}(X_1)^2 - \zeta^{\text{III}}(X_0X_1) - \zeta^{\text{III}}(X_1X_0) = 0$

TABLE 2. Explicit set of relation equivalent to III<sub>KZ</sub> in degree 2



Monomial	Relations
$X_{2,4}X_{2,3}X_{1,2}$	$-2\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) = 0$
$X_{3,4}X_{2,3}X_{1,2}$	$-2\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) = 0$
$X_{2,4}X_{3,4}X_{2,4}$	$2\zeta^{\text{III}}(X_0X_0X_1) + \zeta^{\text{III}}(X_0X_1X_0) = 0$
$X_{3,4}X_{2,4}X_{2,3}$	$-2\zeta^{\text{III}}(X_0X_0X_1) - 2\zeta^{\text{III}}(X_0X_1X_0) - 2\zeta^{\text{III}}(X_1X_0X_0) = 0$
$X_{2,4}X_{1,2}X_{2,3}$	$-\zeta^{\text{III}}(X_0X_1X_0) - 2\zeta^{\text{III}}(X_1X_0X_0) = 0$
$X_{3,4}X_{1,2}X_{2,3}$	$-\zeta^{\text{III}}(X_0X_1X_0) - 2\zeta^{\text{III}}(X_1X_0X_0) = 0$
$X_{2,4}X_{2,4}X_{1,2}$	$-\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) - \zeta^{\text{III}}(X_1X_0X_0) = 0$
$X_{3,4}X_{2,3}X_{2,3}$	$-\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) - \zeta^{\text{III}}(X_1X_0X_0) = 0$
$\mathbf{X}_{3,4}\mathbf{X}_{2,4}\mathbf{X}_{2,4}$	$-\zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_0\mathbf{X}_1) - \zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_1\mathbf{X}_0) - \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_0\mathbf{X}_0) = 0$
$X_{3,4}X_{3,4}X_{1,2}$	$-\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) - \zeta^{\text{III}}(X_1X_0X_0) = 0$
$X_{4,5}X_{4,5}X_{2,3}$	$-\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) - \zeta^{\text{III}}(X_1X_0X_0) = 0$
$\mathbf{X}_{1,2}\mathbf{X}_{2,3}\mathbf{X}_{2,3}$	$\zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_1\mathbf{X}_1) - \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_0\mathbf{X}_0) = 0$
$X_{2,3}X_{1,2}X_{1,2}$	$\zeta^{\text{III}}(X_0X_1X_1) - \zeta^{\text{III}}(X_1X_0X_0) = 0$
$\mathbf{X}_{3,4}\mathbf{X}_{4,5}\mathbf{X}_{4,5}$	$\zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_1\mathbf{X}_1) - \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_0\mathbf{X}_0) = 0$
$\mathbf{X}_{4,5}\mathbf{X}_{2,4}\mathbf{X}_{2,4}$	$\zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_1\mathbf{X}_1) - \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_0\mathbf{X}_0) = 0$
$X_{4,5}X_{3,4}X_{3,4}$	$\zeta^{\text{III}}(X_0X_1X_1) - \zeta^{\text{III}}(X_1X_0X_0) = 0$
$X_{2,4}X_{2,4}X_{3,4}$	$\zeta^{\text{III}}(X_1X_0X_0) - \zeta^{\text{III}}(X_0X_0X_1) = 0$
$X_{2,4}X_{3,4}X_{2,3}$	$2\zeta^{\text{III}}(X_0X_0X_1) + 2\zeta^{\text{III}}(X_0X_1X_0) + 2\zeta^{\text{III}}(X_1X_0X_0) = 0$
$X_{1,2}X_{2,3}X_{1,2}$	$\zeta^{\text{III}}(X_1X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) = 0$
$X_{2,3}X_{1,2}X_{2,3}$	$\zeta^{\text{III}}(X_1X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) = 0$
$X_{2,4}X_{4,5}X_{2,4}$	$\zeta^{\text{III}}(X_1X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) = 0$
$X_{3,4}X_{4,5}X_{3,4}$	$\zeta^{\text{III}}(X_1X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) = 0$
$X_{4,5}X_{3,4}X_{4,5}$	$\zeta^{\text{III}}(X_1X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) = 0$
$X_{4,5}X_{3,4}X_{2,3}$	$2\zeta^{\text{III}}(X_0X_1X_1) + \zeta^{\text{III}}(X_1X_0X_1) = 0$
$X_{4,5}X_{2,4}X_{2,3}$	$-\zeta^{\text{III}}(X_0X_1X_0) + 2\zeta^{\text{III}}(X_0X_1X_1) - 2\zeta^{\text{III}}(X_1X_0X_0) + \zeta^{\text{III}}(X_1X_0X_1) = 0$
$X_{4,5}X_{2,4}X_{4,5}$	$-\zeta^{\text{III}}(X_0X_1X_0) - 2\zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{4,5}X_{2,4}X_{3,4}$	$-\zeta^{\text{III}}(X_0X_1X_0) + \zeta^{\text{III}}(X_0X_1X_1) - \zeta^{\text{III}}(X_1X_0X_0) - 2\zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{2,4}X_{4,5}X_{1,2}$	$-\zeta^{\text{III}}(X_1X_0X_1) - 2\zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{3,4}X_{2,4}X_{3,4}$	$-2\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) - \zeta^{\text{III}}(X_1X_0X_1) - 2\zeta^{\text{III}}(X_1X_1X_0) = 0$

TABLE 3. Explicit set of relation equivalent to  $\text{III}_{\text{KZ}}$  in degree 3 where we already have used the relations  $\zeta^{\text{III}}(X_0^k) = \zeta^{\text{III}}(X_1^k) = 0$ .

Monomial	Relations
$X_{2,4}X_{3,4}X_{1,2}$	$-\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) - \zeta^{\text{III}}(X_1X_0X_0)$ $-\zeta^{\text{III}}(X_1X_0X_1) - 2\zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{3,4}X_{2,4}X_{4,5}$	$\zeta^{\text{III}}(X_1X_0X_0) - \zeta^{\text{III}}(X_1X_1X_0) = 0$
$\mathbf{X}_{1,2}\mathbf{X}_{1,2}\mathbf{X}_{2,3}$	$\zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_1\mathbf{X}_0) - \zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_0\mathbf{X}_1) = 0$
$X_{2,3}X_{2,3}X_{1,2}$	$\zeta^{\text{III}}(X_1X_1X_0) - \zeta^{\text{III}}(X_0X_0X_1) = 0$
$\mathbf{X}_{3,4}\mathbf{X}_{3,4}\mathbf{X}_{4,5}$	$\zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_1\mathbf{X}_0) - \zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_0\mathbf{X}_1) = 0$
$X_{4,5}X_{4,5}X_{2,4}$	$\zeta^{\text{III}}(X_1X_1X_0) - \zeta^{\text{III}}(X_0X_0X_1) = 0$
$X_{4,5}X_{4,5}X_{3,4}$	$\zeta^{\text{III}}(X_1X_1X_0) - \zeta^{\text{III}}(X_0X_0X_1) = 0$
$X_{4,5}X_{3,4}X_{2,4}$	$\zeta^{\text{III}}(X_0X_1X_0) + \zeta^{\text{III}}(X_0X_1X_1) + \zeta^{\text{III}}(X_1X_1X_0) = 0$
$\mathbf{X}_{2,4}\mathbf{X}_{4,5}\mathbf{X}_{4,5}$	$\zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_1\mathbf{X}_0) - \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_0\mathbf{X}_0) = 0$
$X_{2,4}X_{2,4}X_{4,5}$	$\zeta^{\text{III}}(X_0X_1X_0) + \zeta^{\text{III}}(X_1X_0X_0) + \zeta^{\text{III}}(X_1X_1X_0) = 0$
$\mathbf{X}_{2,4}\mathbf{X}_{3,4}\mathbf{X}_{3,4}$	$\zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_0\mathbf{X}_1) + \zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_1\mathbf{X}_0) - \zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_1\mathbf{X}_1)$ $+ \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_0\mathbf{X}_0) + \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_1\mathbf{X}_0) = 0$
$X_{2,4}X_{1,2}X_{1,2}$	$\zeta^{\text{III}}(X_0X_1X_1) + \zeta^{\text{III}}(X_1X_0X_1) + \zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{3,4}X_{1,2}X_{1,2}$	$\zeta^{\text{III}}(X_0X_1X_1) + \zeta^{\text{III}}(X_1X_0X_1) + \zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{3,4}X_{3,4}X_{2,3}$	$\zeta^{\text{III}}(X_0X_1X_1) + \zeta^{\text{III}}(X_1X_0X_1) + \zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{4,5}X_{2,3}X_{2,3}$	$\zeta^{\text{III}}(X_0X_1X_1) + \zeta^{\text{III}}(X_1X_0X_1) + \zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{3,4}X_{4,5}X_{2,4}$	$-\zeta^{\text{III}}(X_0X_1X_0) - \zeta^{\text{III}}(X_1X_0X_0) + \zeta^{\text{III}}(X_1X_0X_1)$ $+ \zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{3,4}X_{3,4}X_{2,4}$	$\zeta^{\text{III}}(X_0X_0X_1) + \zeta^{\text{III}}(X_0X_1X_1) - \zeta^{\text{III}}(X_1X_0X_0)$ $+ \zeta^{\text{III}}(X_1X_0X_1) + \zeta^{\text{III}}(X_1X_1X_0) = 0$
$\mathbf{X}_{2,4}\mathbf{X}_{4,5}\mathbf{X}_{3,4}$	$\zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_0\mathbf{X}_0) + \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_0\mathbf{X}_1) + \zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_1\mathbf{X}_0) = 0$
$\mathbf{X}_{2,4}\mathbf{X}_{3,4}\mathbf{X}_{4,5}$	$\zeta^{\text{III}}(\mathbf{X}_0\mathbf{X}_1\mathbf{X}_0) + 2\zeta^{\text{III}}(\mathbf{X}_1\mathbf{X}_1\mathbf{X}_0) = 0$
$X_{3,4}X_{4,5}X_{2,3}$	$\zeta^{\text{III}}(X_1X_0X_1) + 2\zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{4,5}X_{2,4}X_{1,2}$	$\zeta^{\text{III}}(X_1X_0X_1) + 2\zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{3,4}X_{2,4}X_{1,2}$	$-\zeta^{\text{III}}(X_0X_0X_1) - \zeta^{\text{III}}(X_0X_1X_0) - \zeta^{\text{III}}(X_1X_0X_0)$ $+ \zeta^{\text{III}}(X_1X_0X_1) + 2\zeta^{\text{III}}(X_1X_1X_0) = 0$
$X_{2,4}X_{4,5}X_{2,3}$	$\zeta^{\text{III}}(X_0X_1X_0) + 2\zeta^{\text{III}}(X_1X_0X_0) + \zeta^{\text{III}}(X_1X_0X_1)$ $+ 2\zeta^{\text{III}}(X_1X_1X_0) = 0$

TABLE 4. Explicit set of relation equivalent to  $\text{III}_{\text{KZ}}$  in degree 3 where we already have used the relations  $\zeta^{\text{III}}(X_0^k) = \zeta^{\text{III}}(X_1^k) = 0$ .

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