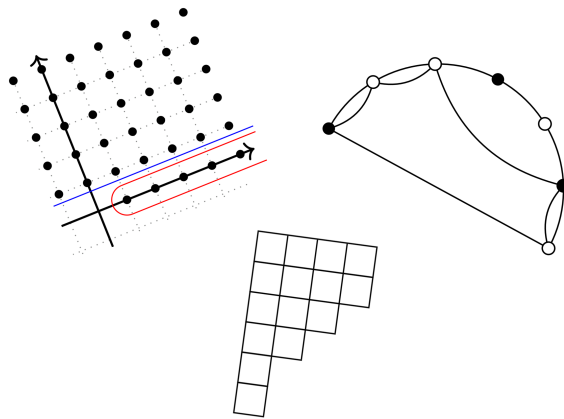


Multiple Eisenstein series and q -analogues of multiple zeta values



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Henrik Bachmann

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Gutachter:

Prof. Dr. Ulf Kühn

Prof. Dr. Don Zagier

Prof. Dr. Wadim Zudilin

Für meine Eltern ♡

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Introduction

This thesis studies a specific connection of multiple zeta values and modular forms given by multiple Eisenstein series. It is a cumulative thesis consisting of four works, [BK],[BT],[Ba2] and [BK2], that can be found in the appendices A, B, C and D respectively. This text is an example-driven overview and summary of the results obtained in these works. It is intended to be submitted as a survey article in the Proceedings of the 2014 ICMAT Research Trimester "Multiple Zeta Values, Multiple Polylogarithms, and Quantum Field Theory". It shall serve as an introduction and motivation for the above mentioned papers¹. Most of the proofs of the main theorems therefore will be omitted.

Multiple zeta values are real numbers that are natural generalizations of the Riemann zeta values. These are defined for integers $s_1 \geq 2$ and $s_2, \dots, s_l \geq 1$ by

$$\zeta(s_1, \dots, s_l) := \sum_{n_1 > n_2 > \dots > n_l > 0} \frac{1}{n_1^{s_1} \dots n_l^{s_l}}.$$

Such real numbers were already studied by Euler in the cases $l = 1$ and $l = 2$ in the 18th century. Because of their occurrence in various fields of mathematics and theoretical physics, the multiple zeta values had a comeback in the mathematical and physical research community in the late 1990s due to works by several people such as D. Broadhurst, F. Brown, P. Deligne, H. Furusho, A. Goncharov, M. Hoffman, M. Kaneko, D. Zagier et al.. Denote the \mathbb{Q} -vector space of all multiple zeta values of weight k by

$$\mathcal{MZ}_k := \left\langle \zeta(s_1, \dots, s_l) \mid s_1 + \dots + s_l = k \text{ and } l > 0 \right\rangle_{\mathbb{Q}}$$

and write \mathcal{MZ} for the space of all multiple zeta values. It is of central interest to understand the \mathbb{Q} -linear relations between these numbers. The first one is given by $\zeta(2, 1) = \zeta(3)$ and several ways are known to prove this relation ([BB]). Using the representation of multiple

¹The versions in the appendix are the most recent ones and may differ from those available in the arxiv.

zeta values as an ordered sum as above, their product can be written as a linear combination of multiple zeta values of the same weight, i.e. the space \mathcal{MZ} has the structure of a \mathbb{Q} -algebra. For example it is

$$\zeta(2) \cdot \zeta(3) = \zeta(2, 3) + \zeta(3, 2) + \zeta(5), \quad (0.1)$$

$$\zeta(3) \cdot \zeta(2, 1) = \zeta(3, 2, 1) + \zeta(2, 3, 1) + \zeta(2, 1, 3) + \zeta(5, 1) + \zeta(2, 4). \quad (0.2)$$

This way to express the product, which will be studied in Chapter 1 in more detail, is called the stuffle product (also named harmonic product). Besides this, a representation of multiple zeta values as iterated integrals yields another way to express the product of two multiple zeta values, which is called the shuffle product. For the above examples, this is given by

$$\zeta(2) \cdot \zeta(3) = \zeta(2, 3) + 3\zeta(3, 2) + 6\zeta(4, 1), \quad (0.3)$$

$$\zeta(3) \cdot \zeta(2, 1) = \zeta(2, 1, 3) + \zeta(2, 2, 2) + 2\zeta(2, 3, 1) + 2\zeta(3, 1, 2) + 5\zeta(3, 2, 1) + 9\zeta(4, 1, 1). \quad (0.4)$$

Since (0.1) and (0.3) are two different expressions for the product $\zeta(2) \cdot \zeta(3)$, we obtain the linear relation $\zeta(5) = 2\zeta(3, 2) + 6\zeta(4, 1)$. These relations are called the double shuffle relations. Conjecturally all \mathbb{Q} -linear relations between multiple zeta values can be proven by using an extended version of these types of relations. Often relations between multiple zeta values are not proven by using double shuffle relations, since there are easier ways to prove them in some cases. The relation $\zeta(4) = \zeta(2, 1, 1)$ for example, has an easy proof using the iterated integral expressions for multiple zeta values. A famous result of Euler is that every even zeta value $\zeta(2k)$ is a rational multiple of π^{2k} . For example, we have

$$\zeta(2)^2 = \frac{5}{2}\zeta(4), \quad \zeta(4)^2 = \frac{7}{6}\zeta(8), \quad \zeta(6)^2 = \frac{715}{691}\zeta(12). \quad (0.5)$$

The relations (0.5) can also be proven using the double shuffle relations, but for general k there is no explicit proof of Eulers relations using only double shuffle relations so far.

Since the double shuffle relations preserve the weight it is conjectured that the space \mathcal{MZ} is a direct sum of the \mathcal{MZ}_k , i.e. there are no relations between multiple zeta values of different weight.

Surprisingly, there are several connections of these numbers to modular forms for the full modular group $\mathrm{SL}_2(\mathbb{Z})$. Recall that modular forms are holomorphic functions in the complex upper half-plane fulfilling certain functional equations. One of the most famous connections between multiple zeta values and modular forms is established by the Broadhurst-Kreimer conjecture.

Conjecture 1. (Broadhurst-Kreimer conjecture) The generating series of the dimension $\dim_{\mathbb{Q}}(\mathcal{MZ}_{k,l})$ of weight k multiple zeta values of length l modulo lower lengths can be written as

$$\sum_{\substack{k \geq 0 \\ l \geq 0}} \dim_{\mathbb{Q}}(\mathcal{MZ}_{k,l}) X^k Y^l = \frac{1 + \mathbb{E}(X)Y}{1 - \mathbb{O}(X)Y + \mathbb{S}(X)Y^2 - \mathbb{S}(X)Y^4},$$

where

$$\mathbb{E}(X) = \frac{X^2}{1 - X^2}, \quad \mathbb{O}(X) = \frac{X^3}{1 - X^2}, \quad \mathbb{S}(X) = \frac{X^{12}}{(1 - X^4)(1 - X^6)}.$$

The connection to modular forms arises here, since $\mathbb{S}(X) = \sum_{k \geq 0} \dim S_k(\mathrm{SL}_2(\mathbb{Z})) X^k$ is the generating function of the dimensions of cusp forms for the full modular group. In the formula of the Broadhurst-Kreimer conjecture, one can see that cusp forms give rise to relations between double zeta values, i.e. multiple zeta values in the length $l = 2$ case. For example in weight 12, the first weight in which non-trivial cusp forms exist, there is the following famous relation

$$\frac{5197}{691} \zeta(12) = 168 \zeta(5, 7) + 150 \zeta(7, 5) + 28 \zeta(9, 3). \quad (0.6)$$

Even though our focus does not lie on the Broadhurst-Kreimer conjecture, the concept of obtaining relations of multiple zeta values by cusp forms also appears in our context of multiple Eisenstein series and q -analogues of multiple zeta values. It is known that every modular form for the full modular group can be written as a polynomial in classical Eisenstein series. These are for even $k > 0$ given by

$$G_k(\tau) = \frac{1}{2} \sum_{\substack{(m,n) \in \mathbb{Z}^2 \\ (m,n) \neq (0,0)}} \frac{1}{(m\tau + n)^k} = \zeta(k) + \frac{(-2\pi i)^k}{(k-1)!} \sum_{n=1}^{\infty} \sigma_{k-1}(n) q^n,$$

where $\tau \in \mathbb{H}$ is an element in the upper half-plane, $q = \exp(2\pi i \tau)$ and $\sigma_k(n) = \sum_{d|n} d^k$ denotes the classical divisor-sum. In [GKZ] the authors introduced a direct connection of modular forms to double zeta values. They defined double Eisenstein series $G_{s_1, s_2} \in \mathbb{C}[[q]]$ which are a length two generalization of classical Eisenstein series and which are given by a double sum over ordered lattice points. These functions have a Fourier expansion given by sums of products of multiple zeta values and certain q -series with the double zeta value $\zeta(s_1, s_2)$ as their constant term. In [Ba], the author treated the multiple cases and calculated the Fourier expansion of multiple Eisenstein series $G_{s_1, \dots, s_l} \in \mathbb{C}[[q]]$. The

result of [Ba] was that the Fourier expansion of multiple Eisenstein series is again a \mathcal{MZ} -linear combination of multiple zeta values and the q -series $g_{t_1, \dots, t_m} \in \mathbb{C}[[q]]$ defined by $g_{t_1, \dots, t_m}(\tau) := (-2\pi i)^{t_1 + \dots + t_m} [t_1, \dots, t_m]$ with $q = e^{2\pi i \tau}$ and

$$[t_1, \dots, t_m] := \sum_{\substack{u_1 > \dots > u_m > 0 \\ v_1, \dots, v_m > 0}} \frac{v_1^{t_1-1} \dots v_m^{t_m-1}}{(t_1-1)! \dots (t_m-1)!} \cdot q^{u_1 v_1 + \dots + u_m v_m}.$$

Theorem 2. ([Ba]) For $s_1, \dots, s_l \geq 2$ the multiple Eisenstein series G_{s_1, \dots, s_l} can be written as a \mathcal{MZ} -linear combination of the above functions g_{t_1, \dots, t_m} .

For example:

$$\begin{aligned} G_{3,2,2}(\tau) = & \zeta(3, 2, 2) + \left(\frac{54}{5} \zeta(2, 3) + \frac{51}{5} \zeta(3, 2) \right) g_2(\tau) + \frac{16}{3} \zeta(2, 2) g_3(\tau) \\ & + 3 \zeta(3) g_{2,2}(\tau) + 4 \zeta(2) g_{3,2}(\tau) + g_{3,2,2}(\tau). \end{aligned}$$

The starting point of this thesis was the fact that there are more multiple zeta values than multiple Eisenstein series, since $\zeta(s_1, \dots, s_l)$ exists for all $s_1 \geq 2, s_2, \dots, s_l \geq 1$ and the G_{s_1, \dots, s_l} just exists when all $s_j \geq 2$. The main objective was to answer the following question

Question 1. *What is a "good" definition of a "regularized" multiple Eisenstein series, such that for each multiple zeta value $\zeta(s_1, \dots, s_l)$ with $s_1 > 1, s_2, \dots, s_l \geq 1$ there is a q -series*

$$G_{s_1, \dots, s_l}^{reg} = \zeta(s_1, \dots, s_l) + \sum_{n>0} a_n q^n \in \mathbb{C}[[q]]$$

with this multiple zeta value as the constant term in its Fourier expansion and which equals the multiple Eisenstein series in the cases $s_1, \dots, s_l \geq 2$?

By "good" we mean that these regularized multiple Eisenstein series should have the same, or at least as close as possible, algebraic structure similar to multiple zeta values. Our answer to this question was approached in several steps which will be described in the following i)-iii). First i) the algebraic structure of the functions g was studied. During this investigation, it turned out, that these objects, or more precisely the q -series $[s_1, \dots, s_l]$ are very interesting objects in their own right. It turned out that in order to understand their algebraic structure it was necessary to study a more general class of q -series, called bi-brackets in ii). The results on bi-brackets and brackets then were used, together with a beautiful connection of the multiple Eisenstein series to the coproduct structure of formal

iterated integrals, to answer the above question in iii).

i) To answer Question 1, the algebraic structure of the functions g , or more precisely the algebraic structure of the q -series $[s_1, \dots, s_l]$, was studied in [BK]. It turned out that these q -series, whose coefficients are given by weighted sums over partitions of n , are, independently of their appearance in the Fourier expansion of multiple Eisenstein series, very interesting objects in their own right. We will denote the \mathbb{Q} -vector space spanned by all these brackets and the constant 1 by \mathcal{MD} . Since we also include the rational numbers, the normalized Eisenstein series $\tilde{G}_k(\tau) := (-2\pi i)^{-k} G_k(\tau)$ are contained in \mathcal{MD} . For example, we have

$$\tilde{G}_2 = -\frac{1}{24} + [2], \quad \tilde{G}_4 = \frac{1}{1440} + [4], \quad \tilde{G}_6 = -\frac{1}{60480} + [6].$$

The algebraic structure of the space \mathcal{MD} was studied in [BK] and one of the main results was the following

Theorem 3. ([BK]) The \mathbb{Q} -vector space spanned by all brackets, equipped with the usual multiplication of formal q -series, is a \mathbb{Q} -algebra, containing the algebra of modular forms with rational coefficients as a subalgebra.

In fact, the product satisfies a quasi-shuffle product and the notion of quasi-shuffle products will be made precise in Section 2.1. Roughly speaking, this means that the product of two brackets can be expressed as a linear combination of brackets similar to the stuffle product (0.1),(0.2) of multiple zeta values. For example we will see that

$$\begin{aligned} [2] \cdot [3] &= [3, 2] + [2, 3] + [5] - \frac{1}{12}[3], \\ [3] \cdot [2, 1] &= [3, 2, 1] + [2, 3, 1] + [2, 1, 3] + [5, 1] + [2, 4] + \frac{1}{12}[2, 2] - \frac{1}{2}[2, 3] - \frac{1}{12}[3, 1], \end{aligned}$$

i.e. up to the lower weight term $-\frac{1}{12}[3]$ and $\frac{1}{12}[2, 2] - \frac{1}{2}[2, 3] - \frac{1}{12}[3, 1]$ this looks exactly like (0.1),(0.2). One might ask if there is also a product structure, which corresponds to the shuffle product (0.3) of multiple zeta values. It turned out that for the lowest length case, this has to do with the differential operator $d = q \frac{d}{dq}$. In [BK], it was shown that

$$[2] \cdot [3] = [2, 3] + 3[3, 2] + 6[4, 1] - 3[4] + d[3], \tag{0.7}$$

which, again up to the term $-3[4] + d[3]$, looks exactly like the shuffle product (0.3) of multiple zeta values. In particular it follows that $d[3]$ is again in the space \mathcal{MD} and in general it was shown that

Theorem 4. ([BK]) The operator $d = q \frac{d}{dq}$ is a derivation on \mathcal{MD} .

ii) Equation (0.7) above was the motivation to study a larger class of q -series, which will be called bi-brackets. While the quasi-shuffle product of brackets also exists in higher length, the second expression for the product, corresponding to the shuffle product, does not appear in higher length if one just allows derivatives as "error terms". The bi-brackets can be seen as a generalization of the derivative of brackets. For $s_1, \dots, s_l \geq 1$, $r_1, \dots, r_l \geq 0$ we define these bi-brackets by

$$\left[\begin{matrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{matrix} \right] := \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \frac{u_1^{r_1}}{r_1!} \cdots \frac{u_l^{r_l}}{r_l!} \cdot \frac{v_1^{s_1-1} \cdots v_l^{s_l-1}}{(s_1-1)! \cdots (s_l-1)!} \cdot q^{u_1 v_1 + \dots + u_l v_l} \in \mathbb{Q}[[q]].$$

In the case $r_1 = \dots = r_l = 0$ these are just ordinary brackets. The products of these seemingly larger class of q -series have two representations similar to the stuffle and shuffle product of multiple zeta values in arbitrary length. For our example, the analog of the shuffle product (0.4) for brackets can now be expressed as

$$\begin{aligned} [3] \cdot [2, 1] &= [2, 1, 3] + [2, 2, 2] + 2[2, 3, 1] + 2[3, 1, 2] + 5[3, 2, 1] + 9[4, 1, 1] \\ &+ \begin{bmatrix} 2, 3 \\ 0, 1 \end{bmatrix} + 2 \begin{bmatrix} 3, 2 \\ 0, 1 \end{bmatrix} + 3 \begin{bmatrix} 4, 1 \\ 1, 0 \end{bmatrix} - [2, 3] - 2[3, 2] - 6[4, 1]. \end{aligned}$$

We will see in Section 3.2 that these double shuffle structure can be described, using the so called partition relation, in a nice combinatorial way. This gives a large family of linear relations between bi-brackets. In fact numerical calculations show that there are so many relations, that we have the following surprising conjecture

Conjecture 5. Every bi-bracket can be written in terms of brackets, i.e. $\mathcal{MD} = \mathcal{BD}$.

Using the algebraic structure of the space of bi-brackets, we now review the definition of shuffle brackets $[s_1, \dots, s_l]^\sqcup$ and stuffle $[s_1, \dots, s_l]^*$ version of the ordinary brackets as certain linear combination of bi-brackets as introduced in [Ba2]. These objects fulfill the same shuffle and stuffle products as multiple zeta values respectively. Both constructions use the theory of quasi-shuffle algebras developed by Hoffman in [H]. We summarize the results in the following Theorem.

Theorem 6. ([Ba2])

- i) The space \mathcal{BD} spanned by all bi-brackets $\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix}$ forms a \mathbb{Q} -algebra containing the space of (quasi-)modular forms and the space \mathcal{MD} of brackets as subalgebras. There are two ways to express the product of two bi-brackets which correspond to the stuffle and shuffle product of multiple zeta values.

-
- ii) There are two subalgebras $\mathcal{MD}^{\sqcup} \subset \mathcal{BD}$ and $\mathcal{MD}^* \subset \mathcal{MD}$ spanned by elements $[s_1, \dots, s_l]^{\sqcup}$ and $[s_1, \dots, s_l]^*$ which fulfill the shuffle and stuffle products, respectively, and which are in the length one case given by the bracket $[s_1]$.

For example, similarly to the relation between multiple zeta values above, we have

$$[2, 3]^* + [3, 2]^* + [5] = [2] \cdot [3] = [2, 3]^{\sqcup} + 3[3, 2]^{\sqcup} + 6[4, 1]^{\sqcup}.$$

iii) A particular reason for studying the $[s_1, \dots, s_l]^{\sqcup}$ is due to their use in the regularization of multiple Eisenstein series, i.e. they are needed in the answer of the original Question 1. This was implicitly done in [BT] by proving an explicit connection of the Fourier expansion of multiple Eisenstein series to the coproduct on formal iterated integrals introduced by Goncharov in [G]. This connection was already known to the authors of [GKZ] in the length two case. Without knowing this connection, it was then rediscovered independently by the authors of [BT] during a research stay of the second author at the DFG Research training Group 1670 at the University of Hamburg in 2014. The result of this research stay was the work [BT], in which the authors used the above-mentioned connection to give a definition of the shuffle regularized multiple Eisenstein series. Later, the present author combined the result of [BT] and the algebraic structure of bi-brackets to give a more explicit definition of shuffle regularized multiple Eisenstein series using bi-brackets in [Ba2].

Formal iterated integrals are symbols $I(a_0; a_1, \dots, a_n; a_{n+1})$ with $a_j \in \{0, 1\}$ that satisfy identities like real iterated integrals. We will write $I(3, 2)$ for $I(1; 00101; 0)$ and we will see that the elements of the form $I(s_1, \dots, s_l)$, obtained in the same way as $I(3, 2)$, form a basis of the space of formal iterated integrals in which we are interested. The space of these integrals has a Hopf algebra structure with the multiplication given by the shuffle product and the coproduct Δ given by an explicit formula, which we will review in Section 4.1. For example it is

$$\Delta(I(3, 2)) = 1 \otimes I(3, 2) + 3I(2) \otimes I(3) + 2I(3) \otimes I(2) + I(3, 2) \otimes 1.$$

Compare this with the Fourier expansion of the double Eisenstein series $G_{3,2}$

$$G_{3,2}(\tau) = \zeta(3, 2) + 3g_2(\tau)\zeta(3) + 2g_3(\tau)\zeta(2) + g_{3,2}(\tau).$$

Since $\Delta(I(s_1, \dots, s_l))$ exists for all $s_1, \dots, s_l \geq 1$, this comparison suggested a definition of shuffle regularized multiple Eisenstein series $G_{s_1, \dots, s_l}^{\sqcup}$ by sending the first component of the coproduct of $I(s_1, \dots, s_l)$ to a $(-2\pi i)$ -multiple of the shuffle bracket and the second component to shuffle regularized multiple zeta values. In [BT], it was proven that this construction returns the original multiple Eisenstein series in the cases $s_1, \dots, s_l \geq 2$. Together with the results on the shuffle brackets in [Ba2], we obtain the following

Theorem 7. ([BT],[Ba2]) For all $s_1, \dots, s_l \geq 1$ there exist shuffle regularized multiple Eisenstein series $G_{s_1, \dots, s_l}^{\sqcup} \in \mathbb{C}[[q]]$ with the following properties:

- i) They are holomorphic functions on the upper half-plane (by setting $q = \exp(2\pi i\tau)$), having a Fourier expansion with the shuffle regularized multiple zeta values as the constant term.
- ii) They fulfill the shuffle product.
- iii) They can be written as a linear combination of multiple zeta values, powers of $(-2\pi i)$ and shuffle brackets $[\dots]^{\sqcup} \in \mathcal{BD}$.
- iv) For integers $s_1, \dots, s_l \geq 2$ they equal the multiple Eisenstein series

$$G_{s_1, \dots, s_l}^{\sqcup}(\tau) = G_{s_1, \dots, s_l}(\tau)$$

and therefore they fulfill the stuffle product in these cases.

We now study the \mathbb{Q} -algebra spanned by the G^{\sqcup} and its relation to multiple zeta values. Theorem 7 iv) gives a subset of the double shuffle relations between the G^{\sqcup} , since the stuffle product is just fulfilled for the case $s_1, \dots, s_l \geq 2$. A natural question is, if they also fulfill the stuffle product when some indices s_j are equal to 1. For some cases this was proven in [Ba2]. For example, it was shown, that

$$G_2^{\sqcup} \cdot G_{2,1}^{\sqcup} = G_{2,1,2}^{\sqcup} + 2G_{2,2,1}^{\sqcup} + G_{2,3}^{\sqcup} + G_{4,1}^{\sqcup}. \quad (0.8)$$

The method to prove this was to introduce stuffle regularized multiple Eisenstein series G_{s_1, \dots, s_l}^* , which fulfill the stuffle product by construction and which equal the classical multiple Eisenstein series in the $s_1, \dots, s_l \geq 2$ cases. Since both G^* and G^{\sqcup} can be written in terms of multiple zeta values and bi-brackets, it was possible to compare these two regularization. It was shown that all G^{\sqcup} appearing in (0.8) equal the G^* ones, from which this equation followed. In contrast to the shuffle regularized multiple Eisenstein series

the stuffle regularized ones could not be defined for all $s_1, \dots, s_l \geq 1$. Still, we have the following results:

Theorem 8. ([Ba2]) For all $s_1, \dots, s_l \geq 1$ and $M \geq 1$ there exists $G_{s_1, \dots, s_l}^{*,M} \in \mathbb{C}[[q]]$ with the following properties

- i) They are holomorphic functions on the upper half-plane (by setting $q = \exp(2\pi i\tau)$) having a Fourier expansion with the stuffle regularized multiple zeta values as the constant term.
- ii) They fulfill the stuffle product.
- iii) In the case where the limit $G_{s_1, \dots, s_l}^* := \lim_{M \rightarrow \infty} G_{s_1, \dots, s_l}^{*,M}$ exists, the functions G_{s_1, \dots, s_l}^* are a linear combination of multiple zeta values, powers of $(-2\pi i)$ and bi-brackets.
- iv) For $s_1, \dots, s_l \geq 2$ the G_{s_1, \dots, s_l}^* exist and equal the classical multiple Eisenstein series

$$G_{s_1, \dots, s_l}(\tau) = G_{s_1, \dots, s_l}^*(\tau).$$

It is still an open question which of the extended double shuffle relations of multiple zeta values also hold for the G^{\sqcup} , or equivalently, under what circumstances the product of two G^{\sqcup} can be expressed using the stuffle product formula. Clearly there are some double shuffle relations which cannot hold for multiple Eisenstein series. For example not all of the Euler relations (0.5) are fulfilled, since G_2^2 is not a multiple of G_4 as G_2 is not modular and G_6^2 is not a multiple of G_{12} as there are cusp forms in weight 12. In Section 4.3, we will explain this failure in terms of the double shuffle relations which are satisfied by multiple Eisenstein series.

From the discussion above, we believe that Question 1 got a satisfying answer given by the regularized multiple Eisenstein series G^{\sqcup} and G^* . In order to go back from multiple Eisenstein series to multiple zeta values, one can consider the projection to the constant term. But there is another direct connection of brackets, and therefore also of the subalgebra of modular forms, to multiple zeta values. The brackets can be seen as a q -analogue of multiple zeta values. A q -analogue of multiple zeta values is said to be a q -series which gives back multiple zeta values in the case $q \rightarrow 1$. Define for $k \in \mathbb{N}$ the map $Z_k : \mathbb{Q}[[q]] \rightarrow \mathbb{R} \cup \{\infty\}$ by

$$Z_k(f) = \lim_{q \rightarrow 1} (1 - q)^k f(q).$$

Proposition 9. ([BK, Prop. 6.4]) For $s_1 \geq 2$ and $s_2, \dots, s_l \geq 1$ the map Z_k sends a bracket to the corresponding multiple zeta value, i.e.

$$Z_k([s_1, \dots, s_l]) = \begin{cases} \zeta(s_1, \dots, s_l), & s_1 + \dots + s_l = k, \\ 0, & s_1 + \dots + s_l < k. \end{cases}$$

Since every relation of multiple zeta values in a given weight k is, by Proposition 9, in the kernel of the map Z_k , this kernel was studied in [BK] with the following result

Theorem 10. ([BK, Thm. 1.13])

- i) For any $f \in \mathcal{MD}$ which can be written as a linear combination of brackets with weight $\leq k - 2$, we have $d f \in \ker Z_k$.
- ii) Any cusp form for $\mathrm{SL}_2(\mathbb{Z})$ of weight k is in the kernel of Z_k .

We give an example for Theorem 10 ii): Using the theory of brackets (Corollary 2.13) we can prove for the cusp form $\Delta = q \prod_{n>0} (1 - q^n)^{24} \in S_{12}(\mathrm{SL}_2(\mathbb{Z}))$ the representation

$$\begin{aligned} -\frac{1}{2^6 \cdot 5 \cdot 691} \Delta &= 168[5, 7] + 150[7, 5] + 28[9, 3] \\ &+ \frac{1}{1408}[2] - \frac{83}{14400}[4] + \frac{187}{6048}[6] - \frac{7}{120}[8] - \frac{5197}{691}[12]. \end{aligned} \quad (0.9)$$

Letting Z_{12} act on both sides of (0.9) one obtains a new proof for the relation (0.6), i.e.,

$$\frac{5197}{691} \zeta(12) = 168\zeta(5, 7) + 150\zeta(7, 5) + 28\zeta(9, 3).$$

Another reason for studying the enlargement of the brackets given by the bi-brackets is the following: In weight 4 one has the relation of multiple zeta values $\zeta(4) = \zeta(2, 1, 1)$, i.e. it is $[4] - [2, 1, 1] \in \ker Z_4$. But this element can't be written as a linear combination of cusp forms, lower weight brackets or derivatives. But one can show, by using the double shuffle relations of bi-brackets, that

$$[4] - [2, 1, 1] = \frac{1}{2} (d[1] + d[2]) - \frac{1}{3}[2] - [3] + \begin{bmatrix} 2, 1 \\ 1, 0 \end{bmatrix} \quad (0.10)$$

and $\begin{bmatrix} 2, 1 \\ 1, 0 \end{bmatrix} \in \ker Z_4$. The description of the kernel of the map Z_k was in fact our first motivation to study the bi-brackets. Equation (0.10) is also an example for the above mentioned Conjecture 5, since it shows that the bi-bracket $\begin{bmatrix} 2, 1 \\ 1, 0 \end{bmatrix}$ can be written in terms of brackets and therefore is an element in \mathcal{MD} .

Outlook and related work

In the following paragraphs a.)-g.) we would like to mention some related works and give an outlook to open questions.

a.) There are still a lot of open questions concerning multiple Eisenstein series as well as the space of (bi-)brackets. After the above mentioned works [BK],[Ba2] and [BT], we now have a good definition of regularized multiple Eisenstein series given by the G^{\sqcup} . For the structure of the space spanned by these series there are still several open questions, for example

- i) What exactly is the failure of the stuffle product for the G^{\sqcup} and when does it hold?
- ii) For which indices $s_1, \dots, s_l \in \mathbb{N}$ do we have $G_{s_1, \dots, s_r}^{\sqcup}(\tau) = G_{s_1, \dots, s_r}^*(\tau)$? Is there an explicit connection between these two regularizations similar to the regularized multiple zeta values given by the map ρ in [IKZ]?
- iii) What is the dimension of the space of (shuffle) regularised multiple Eisenstein series? Is there an explicit basis similar to the Hoffman basis of multiple zeta values (which is given by all multiple zeta values $\zeta(s_1, \dots, s_l)$ with $s_j \in \{2, 3\}$)?
- iv) Which linear combinations of multiple Eisenstein series are modular forms for $SL_2(\mathbb{Z})$? Is there an explicit way to describe the failure of modularity?
- v) Is the space of multiple Eisenstein series closed under the derivative $d = q \frac{d}{dq}$?
- vi) What is the kernel of the projection to the constant term? Does it consist of more than derivatives and cusp forms?
- vii) Is there a general theory behind the connection of the Fourier expansion of multiple Eisenstein series and the Goncharov coproduct? Can we equip the space of multiple Eisenstein series with a coproduct structure in a useful way?

Especially the last question seems to be interesting since the connection to the coproduct of formal iterated integrals is quite mysterious and it seems that there might be a geometric interpretation for this connection.

b.) Several q -analogues of multiple zeta values were studied in recent years (see for example [Zh],[Ta],[MMEF],[OOZ]). These q -analogues often have a product structure similar to the stuffle product of multiple zeta values. In order to obtain something which corresponds to the shuffle product one usually needs to modify the space and add extra elements. In contrast, the bi-brackets have a nice algebraic structure, since they have analogues for both products in a very natural way which therefore gives a lot of linear relations similar to the double shuffle relations. Numerical experiments suggest that every bi-bracket can be written as a linear combination of brackets and therefore (conjecturally) every relation of bi-brackets gives rise to relations between multiple zeta values by applying the map Z_k .

c.) In the case of multiple zeta values, one way to give upper bounds for the dimension is to study the double shuffle space ([IKZ], [IO]). Similarly, one can study the partition shuffle space

$$\mathbb{P}\mathbb{S}(k-l, l) = \left\{ f \in \mathbb{Q}[X_1, \dots, X_l, Y_1, \dots, Y_l] \mid \deg f = k-l, f|_P - f = f|_{\text{Sh}_j} = 0 \forall j \right\},$$

for bi-brackets, where $|_P$ is the involution given by the partition relation (see Section 3.1, (3.1)) and $|_{\text{Sh}_j}$ is given by the sum of all shuffles of type j similar to the one in [IO]. Counting the number of these polynomials, it is possible to give upper bounds for the dimensions of the space of bi-brackets. This approach therefore enabled us to prove the conjecture $\mathcal{MD} = \mathcal{BD}$ up to weight 7 in a current work in progress ([BK3]). Therefore, considering the space $\mathbb{P}\mathbb{S}(k-l, l)$ in more detail might be crucial to understand the structure of bi-brackets.

d.) In this work we were interested in modular forms for the full modular group and consequently studied the level 1 case. In [KT], the authors studied double Eisenstein series and double zeta values of level 2. They also derive the Fourier expansion of these series which involves calculations similar to the level 1 case. One result is that they derive the dimension of the space of double Eisenstein series and give also an upper bound for the dimension of double zeta values of level 2, which involves the dimension of the spaces of cusp forms of level 2. Beside the work on level 2 double Eisenstein series there is also work by H. Yuan and J. Zhao in [YZ] on level N double Eisenstein series. Later on, the same authors also considered a level N version of the brackets in [YZ2].

e.) At the end of [KT], the authors give a proof for an upper bound of the dimension of double zeta values in even weight. We would like to recall this result, since the results

presented in the present work might be able to use these ideas for higher lengths. Consider the space spanned by all normalized double Eisenstein series $(-2\pi i)^{-r-s}G_{r,s}(\tau)$ in even weight $k = r + s$. Denote by π_i the projection of this space to the imaginary part. Using the Fourier expansion of double Eisenstein series, the authors can write down the matrix representation of π_i explicitly. Together with well-known results on period polynomials they obtain

$$\dim_{\mathbb{Q}}\langle \zeta(r, k-r) \mid 2 \leq r \leq k-1 \rangle_{\mathbb{Q}} \leq \frac{k}{2} - 1 - \dim S_k.$$

Due to the Broadhurst-Kreimer conjecture 1, it is conjectured that this is actually an equality. The key fact here is, that it is possible to write down an explicit basis of the imaginary part and the matrix representation of π_i . In order to also obtain upper bounds for the dimensions of multiple zeta values in higher lengths, one might try to use the exact same method as in the length two case. The imaginary part of the (again normalized by the factor $(-2\pi i)^{-k}$) multiple Eisenstein series is more complicated, since it involves the functions g in different length, where it is known that they are not linearly independent anymore. But the algebraic structure of the g , or more precisely of the brackets $[\cdot, \cdot]$, are subject of the current work. It is quite possible that the results on the brackets enable one to study the projection of the imaginary part of multiple Eisenstein series to obtain upper bounds for the Broadhurst-Kreimer conjecture.

f.) The multiple Eisenstein series and the bi-brackets themselves also have connections to counting problems in enumerative geometry:

- i) In [AR] and [R], the author studies q -series $A_k(a) \in \mathbb{Q}[[q]]$ which arises from counting certain types of hyperelliptic curves. One of the results is, that the $A_k(q)$ are contained in the ring of quasi-modular forms. The connection to the brackets is given by the fact that $A_k(q) = [2, \underbrace{\dots, 2}_k]$. The results of [AR] can also be obtained by using an explicit calculation of the Fourier expansion of $G_{2, \dots, 2}$ which will be done in an upcoming work [Ba3].
- ii) In [O] and [QY], the authors connect certain q -analogues of multiple zeta values to Hilbert schemes of points on surfaces. These q -analogues are just particular linear combinations of brackets as explained in [BK2] and Section 5.2.
- iii) The coefficients of bi-brackets also occur naturally when counting flat surfaces [Zo], i.e. certain covers of the torus.

g.) There also exists different "multiple"-versions of classical Eisenstein series. One of them is treated in [BTs], where the authors discuss the series defined by

$$\mathfrak{G}_{2p_1, \dots, 2p_r}(\tau) = \sum_{m \in \mathbb{Z}} \sum_{\substack{n_1 \in \mathbb{Z} \\ (m, n_1) \neq (0, 0)}} \cdots \sum_{\substack{n_r \in \mathbb{Z} \\ (m, n_r) \neq (0, 0)}} \prod_{j=1}^r \frac{1}{(m + n_j \tau)^{2p_j}}$$

for $r \geq 2$ and $p_1, \dots, p_r \geq 1$ and prove (Theorem 2) that

$$\tau^{2(p_1 + \dots + p_r)} \mathfrak{G}_{2p_1, \dots, 2p_r}(\tau) \in \mathbb{Q} \left[\tau^2, \pi^2, G_2(\tau), G_4(\tau), G_6(\tau) \right].$$

The methods used to prove this statement are similar to the methods used in the calculation of the Fourier expansion of multiple Eisenstein series. But besides this, there does not seem to be a direct connection to the multiple Eisenstein series presented here.

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Chapter 1

Multiple Eisenstein series

In this chapter we are going to introduce multiple zeta values and present the multiple Eisenstein series and their Fourier expansion. Especially the construction of the Fourier expansion of multiple Eisenstein series in Section 1.2 was rewritten for this survey. It will be a shortened version of the construction given in [Ba] using results by Bouillot obtained in [Bo]. This chapter is not part of the works [BK], [BK2], [BT] and [BK2]. Before we discuss multiple Eisenstein series, we give a short review of multiple zeta values and their algebraic structure given by the stuffle and shuffle product. In order to describe these two products we will use quasi-shuffle algebras, introduced by Hofmann in [H], which will also be needed later when we deal with the generating series of multiple divisor-sums (brackets) and their generalizations given by the bi-brackets.

1.1 Multiple zeta values and quasi-shuffle algebras

Multiple zeta values are natural generalizations of the Riemann zeta values that are defined¹ for integers $s_1 > 1$ and $s_i \geq 1$ for $i > 1$ by

$$\zeta(s_1, \dots, s_l) := \sum_{n_1 > n_2 > \dots > n_l > 0} \frac{1}{n_1^{s_1} \dots n_l^{s_l}}.$$

We denote the \mathbb{Q} -vector space of all multiple zeta values of weight k by

$$\mathcal{MZ}_k := \left\langle \zeta(s_1, \dots, s_l) \mid s_1 + \dots + s_l = k \text{ and } l > 0 \right\rangle_{\mathbb{Q}}.$$

¹Some authors use the opposite convention $0 < n_1 < \dots < n_l$ in the definition of multiple zeta values. This is in particular the case for the work [BT], where this opposite convention is used for multiple zeta values and multiple Eisenstein series.

It is well known that the product of two multiple zeta values can be written as a linear combination of multiple zeta values of the same weight by using the stuffle or shuffle relations (See for example [IKZ], [Zu2]). Thus they generate a \mathbb{Q} -algebra \mathcal{MZ} . There are several connections of these numbers to modular forms for the full modular group. In the smallest length the stuffle product reads

$$\begin{aligned}\zeta(s_1) \cdot \zeta(s_2) &= \sum_{n_1 > 0} \frac{1}{n_1^{s_1}} \sum_{n_2 > 0} \frac{1}{n_2^{s_2}} \\ &= \sum_{n_1 > n_2 > 0} \frac{1}{n_1^{s_1} n_2^{s_2}} + \sum_{n_2 > n_1 > 0} \frac{1}{n_1^{s_1} n_2^{s_2}} + \sum_{n_1 = n_2 > 0} \frac{1}{n_1^{s_1 + s_2}} \\ &= \zeta(s_1, s_2) + \zeta(s_2, s_1) + \zeta(s_1 + s_2).\end{aligned}$$

For length 1 times length 2 the same argument gives

$$\begin{aligned}\zeta(s_1) \cdot \zeta(s_2, s_3) &= \zeta(s_1, s_2, s_3) + \zeta(s_2, s_1, s_3) + \zeta(s_2, s_3, s_1) \\ &\quad + \zeta(s_1 + s_2, s_3) + \zeta(s_2, s_1 + s_3).\end{aligned}$$

The second expression for the product, the shuffle product, comes from the iterated integral expression of multiple zeta values. For example it is

$$\zeta(2, 3) = \int_{1 > t_1 > \dots > t_5 > 0} \underbrace{\frac{dt_1}{t_1} \cdot \frac{dt_2}{1-t_2}}_2 \cdot \underbrace{\frac{dt_3}{t_3} \cdot \frac{dt_4}{t_4} \cdot \frac{dt_5}{1-t_5}}_3.$$

Multiplying two of these integrals one obtains again a linear combination of multiple zeta values as for example

$$\zeta(2) \cdot \zeta(3) = \zeta(2, 3) + 3\zeta(3, 2) + 6\zeta(4, 1).$$

More generally the smallest length case is given by

$$\zeta(s_1) \cdot \zeta(s_2) = \sum_{\substack{a+b=s_1+s_2 \\ a>1}} \left(\binom{a-1}{s_1-1} + \binom{a-1}{s_2-1} \right) \zeta(a, b). \quad (1.1)$$

To describe these two product structures precisely we will use the language of quasi-shuffle algebras as introduced in [H].

Definition 1.2. Let A (the alphabet) be a countable set of letters, $\mathbb{Q}A$ the \mathbb{Q} -vector space generated by these letters and $\mathbb{Q}\langle A \rangle$ the noncommutative polynomial algebra over \mathbb{Q} generated by words with letters in A . For a commutative and associative product \diamond on $\mathbb{Q}A$,

$a, b \in A$ and $w, v \in \mathbb{Q}\langle A \rangle$ we define on $\mathbb{Q}\langle A \rangle$ recursively a product by $1 \odot w = w \odot 1 = w$ and

$$aw \odot bv := a(w \odot bv) + b(aw \odot v) + (a \diamond b)(w \odot v). \quad (1.2)$$

By a result of Hoffman ([H, Thm. 2.1]) $(\mathbb{Q}\langle A \rangle, \odot)$ is a commutative \mathbb{Q} -algebra which is called a *quasi-shuffle algebra*.

To describe the stuffle and the shuffle product for multiple zeta values we need to deal with two different alphabets A_{xy} and A_z . The first alphabet is given by $A_{xy} := \{x, y\}$ and we set $\mathfrak{H} = \mathbb{Q}\langle A_{xy} \rangle$ and $\mathfrak{H}^1 = 1 \cdot \mathbb{Q} + \mathfrak{H}y$, with 1 being the empty word. It is easy to see that \mathfrak{H}^1 is generated by the elements $z_j = x^{j-1}y$ with $j \in \mathbb{N}$, i.e. $\mathfrak{H}^1 = \mathbb{Q}\langle A_z \rangle$ with the second alphabet $A_z := \{z_1, z_2, \dots\}$. Additionally, we define $\mathfrak{H}^0 = 1\mathbb{Q} + x\mathfrak{H}y$.

- i) On \mathfrak{H}^1 we have the following quasi-shuffle product with respect to the alphabet A_z , called the *stuffle product*. We denote it by $*$ and define it as the quasi-shuffle product with $z_j \diamond z_i = z_{j+i}$. For $a, b \in \mathbb{N}$ and $w, v \in \mathfrak{H}^1$ we therefore have:

$$z_a w * z_b v = z_a(w * z_b v) + z_b(z_a w * v) + z_{a+b}(w * v).$$

By $(\mathfrak{H}^1, *)$ we denote the corresponding \mathbb{Q} -algebra.

- ii) On the alphabet A_{xy} we define the *shuffle product* as the quasi-shuffle product with $\diamond \equiv 0$, and by (\mathfrak{H}^1, \sqcup) we denote the corresponding \mathbb{Q} -algebra.

It is easy to check that \mathfrak{H}^0 is closed under both products $*$ and \sqcup and therefore we have also the two algebras $(\mathfrak{H}^0, *)$ and (\mathfrak{H}^0, \sqcup) .

By the definition of multiple zeta values as an ordered sum and by the iterated integral expression one obtains algebra homomorphisms $Z : (\mathfrak{H}^0, *) \rightarrow \mathcal{MZ}$ and $Z : (\mathfrak{H}^0, \sqcup) \rightarrow \mathcal{MZ}$ by sending $w = z_{s_1} \dots z_{s_l}$ to $\zeta(w) = \zeta(s_1, \dots, s_l)$, since the words in \mathfrak{H}^0 correspond exactly to the indices for which the multiple zeta values are defined. It is a well known fact, that these algebra homomorphisms can be extended to \mathfrak{H}^1 :

Proposition 1.1. ([IKZ, Prop. 1]) There exist algebra homomorphisms

$$Z^* : (\mathfrak{H}^1, *) \longrightarrow \mathcal{MZ} \quad \text{and} \quad Z^\sqcup : (\mathfrak{H}^1, \sqcup) \longrightarrow \mathcal{MZ},$$

which are uniquely determined by $Z^*(w) = Z^\sqcup(w) = \zeta(w)$ for $w \in \mathfrak{H}^0$ and by their images on the word z_1 , which we set 0 here, i.e. $Z^*(z_1) = Z^\sqcup(z_1) = 0$.

□

1.3 Multiple Eisenstein series and the calculation of their Fourier expansion

The Riemann zeta values appear as the constant term in the Fourier expansion of classical Eisenstein series. These series are defined by

$$G_k(\tau) = \frac{1}{2} \sum_{\substack{(m,n) \in \mathbb{Z}^2 \\ (m,n) \neq (0,0)}} \frac{1}{(m\tau + n)^k}. \quad (1.3)$$

where $k > 2$ is called the weight. Splitting the summation into the parts $m = 0$ and $m \in \mathbb{Z} \setminus 0$ we obtain for even k

$$G_k(\tau) = \frac{1}{2} \sum_{n \neq 0} \frac{1}{n^k} + \sum_{m=1}^{\infty} \left(\sum_{n \in \mathbb{Z}} \frac{1}{(m\tau + n)^k} \right).$$

To calculate the Fourier expansion of the sum on the right, one uses the well known Lipschitz summation formula

$$\sum_{d \in \mathbb{Z}} \frac{1}{(\tau + d)^k} = \frac{(-2\pi i)^k}{(k-1)!} \sum_{m=1}^{\infty} m^{k-1} q^m, \quad (1.4)$$

which is valid for $k > 1$. With (1.4) we obtain

$$G_k(\tau) = \zeta(k) + \frac{(-2\pi i)^k}{(k-1)!} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} n^{k-1} q^{mn} = \zeta(k) + \frac{(-2\pi i)^k}{(k-1)!} \sum_{n=1}^{\infty} \sigma_{k-1}(n) q^n, \quad (1.5)$$

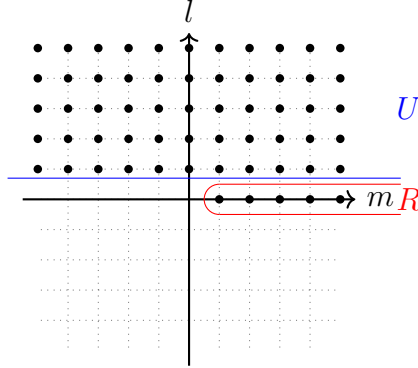
where $\sigma_k(n) = \sum_{d|n} d^k$ denote the divisor-sum. Formula (1.5) also makes sense for odd k but does not give a modular form, since there are no non trivial modular forms of odd weight. The sum in (1.3) vanishes for odd k , therefore instead of summing over the whole lattice, we restrict the summation to the positive lattice points, with positivity coming from an order on the lattice $\mathbb{Z}\tau + \mathbb{Z}$. This in turn will also enable us to give an multiple version of the Eisenstein series in an obvious way.

Let $\Lambda_\tau = \mathbb{Z}\tau + \mathbb{Z}$ be a lattice with $\tau \in \mathbb{H} := \{x + iy \in \mathbb{C} \mid y > 0\}$. We define an order \succ on Λ_τ by setting

$$\lambda_1 \succ \lambda_2 \Leftrightarrow \lambda_1 - \lambda_2 \in P$$

for $\lambda_1, \lambda_2 \in \Lambda_\tau$ and the following set P , which we call the set of positive lattice points

$$P := \{l\tau + m \in \Lambda_\tau \mid l > 0 \vee (l = 0 \wedge m > 0)\} = U \cup R$$



Definition 1.4. For $s_1 \geq 3, s_2, \dots, s_l \geq 2$ we define the *multiple Eisenstein series* of weight $k = s_1 + \dots + s_l$ and length l by

$$G_{s_1, \dots, s_l}(\tau) := \sum_{\substack{\lambda_1 > \dots > \lambda_l > 0 \\ \lambda_i \in \Lambda_\tau}} \frac{1}{\lambda_1^{s_1} \dots \lambda_l^{s_l}}.$$

It is easy to see that these are holomorphic functions in the upper half-plane and that they fulfill the stuffle product, i.e. for example

$$G_3(\tau) \cdot G_4(\tau) = G_{4,3}(\tau) + G_{3,4}(\tau) + G_7(\tau).$$

By definition it is $G_{s_1, \dots, s_l}(\tau + 1) = G_{s_1, \dots, s_l}(\tau)$, i.e. there exists a Fourier expansion of G_{s_1, \dots, s_l} in $q = e^{2\pi i \tau}$. To write down the Fourier expansion of multiple Eisenstein series we need to introduce the following q -series which will be studied in detail in Section 2.1. For $s_1, \dots, s_l \geq 1$ we define

$$[s_1, \dots, s_l] := \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \frac{v_1^{s_1-1} \dots v_l^{s_l-1}}{(s_1-1)! \dots (s_l-1)!} \cdot q^{u_1 v_1 + \dots + u_l v_l} \in \mathbb{Q}[[q]].$$

and write $g_{s_1, \dots, s_l}(\tau) := (-2\pi i)^{s_1, \dots, s_l} [s_1, \dots, s_l]$, which is an holomorphic function in the upper half-plane by setting $q = e^{2\pi i \tau}$.

Theorem 1.2. ([Ba], Fourier expansion) For $s_1 \geq 3, s_2, \dots, s_l \geq 2$ the $G_{s_1, \dots, s_l}(\tau)$ can be written as a \mathcal{MZ} -linear combination of the functions g . More precisely there are rational numbers $\lambda_{r,j} \in \mathbb{Q}$, for $r = (r_1, \dots, r_l)$ and $1 \leq j \leq l-1$, such that (with $k = s_1 + \dots + s_l$)

$$G_{s_1, \dots, s_l}(\tau) = \zeta(s_1, \dots, s_l) + \sum_{\substack{1 \leq j \leq l-1 \\ r_1 + \dots + r_l = k}} \lambda_{r,j} \cdot \zeta(r_1, \dots, r_j) \cdot g_{r_{j+1}, \dots, r_l}(\tau) + g_{s_1, \dots, s_l}(\tau).$$

Even though the proof of this statement is the main result of [Ba] we will give a shortened version of it in the following.

The condition $s_1 \geq 3$ is necessary for the absolute convergence of the sum. Nevertheless we can also allow the case $s_1 = 2$ by using the Eisenstein summation as it was done in [BT] Definition 2.1. This corresponds to the usual way of defining the quasi-modular form G_2 in length one. Since the construction of the Fourier expansion described below uses exactly this Eisenstein summation the Theorem 1.4 is also valid for $s_1 \geq 2$.

For example the triple Eisenstein series $G_{3,2,2}$ can be written as

$$G_{3,2,2}(\tau) = \zeta(3, 2, 2) + \left(\frac{54}{5} \zeta(2, 3) + \frac{51}{5} \zeta(3, 2) \right) g_2(\tau) + \frac{16}{3} \zeta(2, 2) g_3(\tau) \\ + 3\zeta(3)g_{2,2}(\tau) + 4\zeta(2)g_{3,2}(\tau) + g_{3,2,2}(\tau).$$

To derive the Fourier expansion we introduce the following functions, that can be seen as a multiple version of the term $\sum_{n \in \mathbb{Z}} \frac{1}{(x+n)^k}$ appearing in the calculation of the Fourier expansion of classical Eisenstein series.

Definition 1.5. For $s_1, \dots, s_l \geq 2$ we define the multitangent function of length l by

$$\Psi_{s_1, \dots, s_l}(x) = \sum_{\substack{n_1 > \dots > n_l \\ n_i \in \mathbb{Z}}} \frac{1}{(x+n_1)^{s_1} \dots (x+n_l)^{s_l}}.$$

In the case $l = 1$ we also refer to these as monotangent function.

These functions were introduced and studied in detail in [Bo]. One of the main results there, which is crucial for the calculation of the Fourier expansion presented here, is the following theorem which reduces the multitangent functions into monotangent functions.

Theorem 1.3. ([Bo, Thm. 3], Reduction of multitangent into monotangent functions) For $s_1, \dots, s_l \geq 2$ and $k = s_1 + \dots + s_l$ the multitangent function can be written as a \mathcal{MZ} -linear combination of monotangent functions, more precisely there are $c_{k,h} \in \mathcal{MZ}_{k-h}$ such that

$$\Psi_{s_1, \dots, s_l}(x) = \sum_{h=2}^k c_{k-h} \Psi_h(x).$$

Proof. An explicit formula for the coefficients c_k is given in Theorem 3 in [Bo]. The proof uses partial fraction and a non trivial relation between multiple zeta values to argue that

the sum starts at $h = 2$. For example in length two it is

$$\begin{aligned}
 \Psi_{3,2}(x) &= \sum_{m_1 > m_2} \frac{1}{(x + m_1)^3 (x + m_2)^2} \\
 &= \sum_{m_1 > m_2} \left(\frac{1}{(m_1 - m_2)^2 (x + m_1)^3} + \frac{2}{(m_1 - m_2)^3 (x + m_1)^2} + \frac{3}{(m_1 - m_2)^4 (x + m_1)} \right) \\
 &+ \sum_{m_1 > m_2} \left(\frac{1}{(m_1 - m_2)^3 (x + m_2)^2} - \frac{3}{(m_1 - m_2)^4 (x + m_2)} \right) \\
 &= 3\zeta(3)\Psi_2(x) + \zeta(2)\Psi_3(x).
 \end{aligned} \tag{1.6}$$

□

The connection between the functions g and the monotangent functions is given by the following

Proposition 1.4. For $s_1, \dots, s_r \geq 2$ the functions g can be written as an ordered sum of monotangent functions

$$g_{s_1, \dots, s_l}(\tau) = \sum_{m_1 > \dots > m_l > 0} \Psi_{s_1}(m_1\tau) \dots \Psi_{s_r}(m_r\tau).$$

Proof. This follows directly by the Lipschitz formula (1.4) and the definition of the functions g . □

Preparation for the Proof of Theorem 1.4: We will now recall the construction of the Fourier expansion of multiple Eisenstein series introduced in [Ba], in order to prove Theorem 1.4. To calculate the Fourier expansion we rewrite the multiple Eisenstein series as

$$\begin{aligned}
 G_{s_1, \dots, s_l}(\tau) &= \sum_{\lambda_1 > \dots > \lambda_l > 0} \frac{1}{\lambda_1^{s_1} \dots \lambda_l^{s_l}} \\
 &= \sum_{(\lambda_1, \dots, \lambda_l) \in P^l} \frac{1}{(\lambda_1 + \dots + \lambda_l)^{s_1} (\lambda_2 + \dots + \lambda_l)^{s_2} \dots (\lambda_l)^{s_l}}.
 \end{aligned}$$

We decompose the set of tuples of positive lattice points P^l into the 2^l distinct subsets $A_1 \times \dots \times A_l \subset P^l$ with $A_i \in \{R, U\}$ and write

$$G_{s_1, \dots, s_l}^{A_1 \dots A_l}(\tau) := \sum_{(\lambda_1, \dots, \lambda_l) \in A_1 \times \dots \times A_l} \frac{1}{(\lambda_1 + \dots + \lambda_l)^{s_1} (\lambda_2 + \dots + \lambda_l)^{s_2} \dots (\lambda_l)^{s_l}}$$

this gives the decomposition

$$G_{s_1, \dots, s_l} = \sum_{A_1, \dots, A_l \in \{R, U\}} G_{s_1, \dots, s_l}^{A_1 \dots A_l}.$$

In the following we identify the $A_1 \dots A_l$ with words in the alphabet $\{R, U\}$. In length $l = 1$ we have $G_k(\tau) = G_k^R(\tau) + G_k^U(\tau)$ and

$$G_k^R(\tau) = \sum_{\substack{m_1=0 \\ n_1>0}} \frac{1}{(0\tau + n_1)^k} = \zeta(k),$$

$$G_k^U(\tau) = \sum_{\substack{m_1>0 \\ n_1 \in \mathbb{Z}}} \frac{1}{(m_1\tau + n_1)^k} = \sum_{m_1>0} \Psi_k(m_1\tau),$$

where Ψ_k is the monotent function given by

$$\Psi_k(x) = \sum_{n \in \mathbb{Z}} \frac{1}{(x+n)^k}.$$

To calculate the Fourier expansion of G_k^U one uses the Lipschitz formula (1.4). In general the $G_{s_1, \dots, s_l}^{U^l}$ can be written as

$$\begin{aligned} G_{s_1, \dots, s_l}^{U^l}(\tau) &= \sum_{\substack{m_1 > \dots > m_l > 0 \\ n_1, \dots, n_l \in \mathbb{Z}}} \frac{1}{(m_1\tau + n_1)^{s_1} \dots (m_l\tau + n_l)^{s_l}} \\ &= \sum_{m_1 > \dots > m_l > 0} \Psi_{s_1}(m_1\tau) \dots \Psi_{s_l}(m_l\tau) \\ &= \frac{(-2\pi i)^{s_1 + \dots + s_l}}{(s_1 - 1)! \dots (s_l - 1)!} \sum_{\substack{m_1 > \dots > m_l > 0 \\ d_1, \dots, d_l > 0}} d_1^{s_1-1} \dots d_l^{s_l-1} q^{m_1 d_1 + \dots + m_l d_l} \\ &= g_{s_1, \dots, s_l}(\tau). \end{aligned}$$

The other special case $G_{s_1, \dots, s_l}^{R^l}$ can also be written down explicitly:

$$G_{s_1, \dots, s_l}^{R^l}(\tau) = \sum_{\substack{m_1 = \dots = m_l = 0 \\ n_1 > \dots > n_l > 0}} \frac{1}{(0\tau + n_1)^{s_1} \dots (0\tau + n_l)^{s_l}} = \zeta(s_1, \dots, s_l).$$

In length 2 we have $G_{s_1, s_2} = G_{s_1, s_2}^{RR} + G_{s_1, s_2}^{UR} + G_{s_1, s_2}^{RU} + G_{s_1, s_2}^{UU}$ and

$$\begin{aligned} G_{s_1, s_2}^{UR} &= \sum_{\substack{m_1 > 0, m_2 = 0 \\ n_1 \in \mathbb{Z}, n_2 > 0}} \frac{1}{(m_1\tau + n_1)^{s_1} (0\tau + n_2)^{s_2}} \\ &= \sum_{m_1 > 0} \Psi_{s_1}(m_1\tau) \sum_{n_2 > 0} \frac{1}{n_2^{s_2}} = g_{s_1}(\tau) \zeta(s_2), \\ G_{s_1, s_2}^{RU}(\tau) &= \sum_{\substack{m_1 = 0, m_2 > 0 \\ n_1 > n_2 \\ n_i \in \mathbb{Z}}} \frac{1}{(m_1\tau + n_1)^{s_1} (m_1\tau + n_2)^{s_2}} = \sum_{m > 0} \Psi_{s_1, s_2}(m\tau). \end{aligned}$$

1.3. Multiple Eisenstein series and the calculation of their Fourier expansion

In the case G^{UR} we saw that we could write it as G^U multiplied with a zeta value. In general, having a word w of length l ending in the letter R , i.e. there is a word w' ending in U with $w = w'R^r$ and $1 \leq r \leq l$ we can write

$$G_{s_1, \dots, s_l}^w(\tau) = G_{s_1, \dots, s_{l-r}}^{w'}(\tau) \cdot \zeta(s_{l-r+1}, \dots, s_l).$$

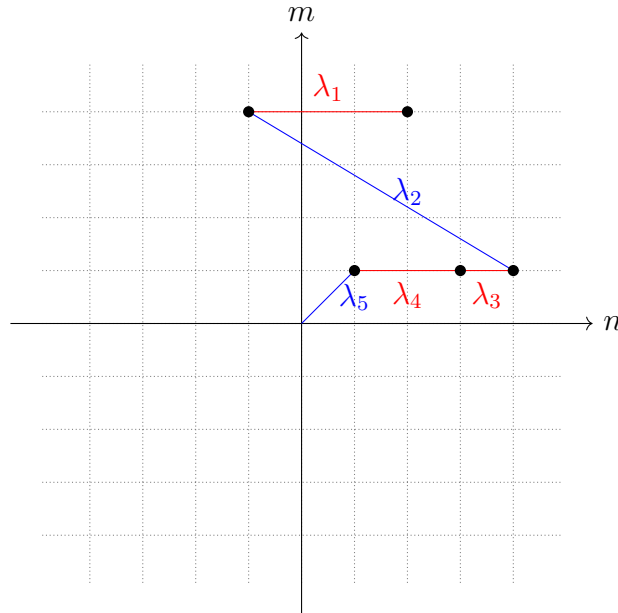
Example: $G_{3,4,5,6,7}^{RUURR} = G_{3,4,5}^{RUU} \cdot \zeta(6, 7)$

Hence one can concentrate on the words ending in U when calculating the Fourier expansion of a multiple Eisenstein series. Let w be a word ending in U then there are integers $r_1, \dots, r_j \geq 0$ with $w = R^{r_1}UR^{r_2}U \dots R^{r_j}U$. With this one can write

$$G_{s_1, \dots, s_l}^w(\tau) = \sum_{m_1 > \dots > m_j > 0} \Psi_{s_1, \dots, s_{r_1+1}}(m_1\tau) \cdot \Psi_{s_{r_1+2}, \dots}(m_2\tau) \dots \Psi_{s_{l-r_j}, \dots, s_l}(m_j\tau).$$

Example: $w = RURRU$

$$G_{s_1, \dots, s_l}^{RURRU} = \sum_{m_1 > m_2 > 0} \Psi_{s_1, s_2}(m_1\tau) \Psi_{s_3, s_4, s_5}(m_2\tau)$$



A summand of $G_{s_1, \dots, s_l}^{RURRU}$.

Proof of Theorem 1.4: For $s_1, \dots, s_l \geq 2$ the Fourier expansion of the multiple Eisenstein series G_{s_1, \dots, s_l} can be computed in the following way

- i) Split up the summation into 2^l distinct parts G_{s_1, \dots, s_l}^w where w are a words in $\{R, U\}$.
- ii) For w being a word ending in R one can write G_{s_1, \dots, s_l}^w as $G_{s_1, \dots}^{w'} \cdot \zeta(\dots, s_l)$ with a word w' ending in U .
- iii) For w being a word ending in U one can write G_{s_1, \dots, s_l}^w as

$$G_{s_1, \dots, s_l}^w(\tau) = \sum_{m_1 > \dots > m_l > 0} \Psi_{s_1, \dots}(m_1 \tau) \dots \Psi_{\dots, s_l}(m_l \tau).$$

- iv) Using the Theorem 1.6 we can write the multitangent functions in iii) as a \mathcal{MZ} -linear combination of monotangents. We therefore just have \mathcal{MZ} -linear combinations with sums of the form

$$\sum_{m_1 > \dots > m_j > 0} \Psi_{k_1}(m_1 \tau) \dots \Psi_{k_j}(m_j \tau) = g_{k_1, \dots, k_l}(\tau) = (-2\pi i)^{k_1 + \dots + k_l} [k_1, \dots, k_l].$$

□

An explicit formula for the Fourier expansion of the multiple Eisenstein series for arbitrary length can be found in [BT] Proposition 2.4. (with a reversed order of indices). Here we just give the Fourier expansion for the length 2 and 3. For this we define for $n_1, n_2, k > 0$ the numbers C_{n_1, n_2}^k by

$$C_{n_1, n_2}^k = (-1)^{n_2} \binom{k-1}{n_2-1} + (-1)^{k-n_1} \binom{k-1}{n_1-1}.$$

Proposition 1.5. i) ([GKZ, Formula (52)], [Ba], [BT]) For $s_1, s_2 \geq 2$ the Fourier expansion of the double Eisenstein series is given by

$$G_{s_1, s_2}(\tau) = \zeta(s_1, s_2) + \zeta(s_2)g_1(\tau) + \sum_{\substack{k_1+k_2=s_1+s_2 \\ k_2, k_2 \geq 2}} C_{s_1, s_2}^{k_2} \zeta(k_2)g_{k_1}(\tau) + g_{s_1, s_2}(\tau).$$

- ii) ([Ba], [BT]) For $s_1, s_2, s_3 \geq 2$ and $k = s_1 + s_2 + s_3$ the Fourier expansion of the triple

Eisenstein series can be written as

$$\begin{aligned}
 G_{s_1, s_2, s_3}(\tau) &= \zeta(s_1, s_2, s_3) + \zeta(s_2, s_3)g_{s_1}(\tau) + \zeta(s_3)g_{s_1, s_2}(\tau) + g_{s_1, s_2, s_3}(\tau) \\
 &+ \zeta(s_3) \sum_{k_1+k_2=s_1+s_2} C_{s_1, s_2}^{k_1} \zeta(k_1)g_{k_2}(\tau) \\
 &+ \sum_{k_1+k_2=s_1+s_2} C_{s_1, s_2}^{k_2} \zeta(k_2)g_{k_1, s_3}(\tau) + \sum_{k_1+k_2=s_2+s_3} C_{s_2, s_3}^{k_2} \zeta(k_2)g_{s_1, k_1}(\tau) \\
 &+ \sum_{k_1+k_2+k_3=k} (-1)^{s_2+s_3} \binom{k_2-1}{s_2-1} \binom{k_3-1}{s_3-1} \zeta(k_3, k_2)g_{k_1}(\tau) \\
 &+ \sum_{k_1+k_2+k_3=k} (-1)^{s_1+s_2+k_2+k_3} \binom{k_2-1}{k_3-1} \binom{k_3-1}{s_2-1} \zeta(k_3, k_2)g_{k_1}(\tau) \\
 &+ (-1)^{s_1+s_3} \sum_{k_1+k_2+k_3=k} (-1)^{k_2} \binom{k_2-1}{s_1-1} \binom{k_3-1}{s_3-1} \zeta(k_3)\zeta(k_2)g_{k_1}(\tau),
 \end{aligned}$$

where in the sums we sum over all $k_i \geq 2$.

□

We finish this section with a closer look at the stuffle product of two Eisenstein series. Since the product of multiple Eisenstein series can be written in terms of the stuffle product it is $G_2 \cdot G_3 = G_{2,3} + G_{3,2} + G_5$. On the other hand we have

$$G_2 \cdot G_3 = (\zeta(2) + g_2)(\zeta(3) + g_3) = \zeta(2)\zeta(3) + \zeta(3)g_2 + \zeta(2)g_3 + g_2 \cdot g_3.$$

and by Proposition 1.8 it is

$$\begin{aligned}
 G_{2,3} &= \zeta(2, 3) - 2\zeta(3)g_2 + \zeta(2)g_3 + g_{2,3}, \\
 G_{3,2} &= \zeta(3, 2) + 3\zeta(3)g_2 + \zeta(2)g_3 + g_{3,2}.
 \end{aligned}$$

In conclusion, we obtain a relation for the product of the g 's namely $g_2 \cdot g_3 = g_{3,2} + g_{2,3} + g_5 + 2\zeta(2)g_3$ and dividing out $(-2\pi i)^5$ we get

$$[2] \cdot [3] = [3, 2] + [2, 3] + [5] - \frac{1}{12}[3].$$

We conclude that a product of the q -series $[s_1, \dots, s_l] \in \mathbb{Q}[[q]]$ has an expression similar to the stuffle product and that conversely, a product structure on these q -series could be used, together with the Fourier expansion, to explain the stuffle product for multiple Eisenstein series.

One might now ask, if the multiple Eisenstein series also "fulfill" the shuffle product. As we saw above the shuffle product of $\zeta(2)$ and $\zeta(3)$ reads

$$\zeta(2) \cdot \zeta(3) = \zeta(2, 3) + 3\zeta(3, 2) + 6\zeta(4, 1) \tag{1.7}$$

and since there is no definition of $G_{4,1}$ this question does not make sense when replacing ζ by G in (1.7). We will see that the understanding of the product structure of the brackets, explained in the next two chapters, together with the Fourier expansion of multiple Eisenstein series will help to answer this question. This will be done by introducing shuffle regularized multiple Eisenstein series G^{\sqcup} in Section 4.2. There we will see that we can replace the ζ in (1.7) by G^{\sqcup} and that the G^{\sqcup} are given by the original G , for the cases in which they are defined.

Chapter 2

Multiple divisor-sums and their generating functions

The classical divisor-sums $\sigma_r(n) = \sum_{d|n} d^r$ have a long history in number theory. They are well-known examples for multiplicative functions and appear in the Fourier expansion of Eisenstein series. This chapter is devoted to a larger class of functions, that can be seen as a multiple version of the divisor-sums and are therefore called multiple divisor-sums. For natural numbers $r_1, \dots, r_l \geq 0$ they are defined by

$$\sigma_{r_1, \dots, r_l}(n) = \sum_{\substack{u_1 v_1 + \dots + u_l v_l = n \\ u_1 > \dots > u_l > 0}} v_1^{r_1} \dots v_l^{r_l}. \quad (2.1)$$

Even though the definition of these arithmetic functions is not complicated and somehow canonical, the author could not find any results on these functions before he started studying them in his master thesis [Ba]. As mentioned in the introduction, the motivation to study them was due to their appearance in the Fourier expansion of multiple Eisenstein series, but as it turned out later in [BK], they are very nice and interesting objects in their own right. Similar to multiple zeta values they fulfill a lot of relations. For example it is

$$\frac{1}{2}\sigma_2(n) = \sigma_{1,0}(n) - \frac{1}{2}\sigma_1(n) + n\sigma_0(n). \quad (2.2)$$

Having objects of this type it is natural to consider their generating functions, which we denote by

$$[s_1, \dots, s_l] := \frac{1}{(s_1 - 1)! \dots (s_l - 1)!} \sum_{n > 0} \sigma_{s_1-1, \dots, s_l-1}(n) q^n$$

and which are, just for the sake of short notations, called brackets. The factorial factors and the "shift" of -1 are natural if one thinks about the Fourier expansion of Eisenstein series. With this notation the relation (2.2) reads as

$$[3] = [2, 1] - \frac{1}{2}[2] + q \frac{d}{dq}[1], \quad (2.3)$$

which can be seen as a counterpart of the relation $\zeta(3) = \zeta(2, 1)$ between multiple zeta values¹.

In this chapter, we want to focus on the algebraic structure of the space spanned by all brackets, which we will denote by \mathcal{MD} . This algebraic structure was studied in [BK]. We will see that the space \mathcal{MD} has the structure of a \mathbb{Q} -algebra and that the product of two brackets can be expressed in terms of brackets in a way that looks similar to the stuffle product of multiple zeta values. The operator $d = q \frac{d}{dq}$ which appears in (2.3) plays an important role in the theory of (quasi-)modular forms. We will see that the space \mathcal{MD} is closed under this operator and that this gives a second way of expressing the product of two brackets in length one similarly to the shuffle product of multiple zeta values. This second product expression in higher length will be discussed in Chapter 3.

2.1 Brackets

Definition 2.2. For any integers $s_1, \dots, s_l > 0$ we define the generating function for the multiple divisor sum $\sigma_{s_1-1, \dots, s_l-1}$ by the formal power series

$$\begin{aligned} [s_1, \dots, s_l] &:= \frac{1}{(s_1 - 1)! \dots (s_l - 1)!} \sum_{n>0} \sigma_{s_1-1, \dots, s_l-1}(n) q^n \\ &= \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \frac{v_1^{s_1-1} \dots v_l^{s_l-1}}{(s_1 - 1)! \dots (s_l - 1)!} \cdot q^{u_1 v_1 + \dots + u_l v_l} \in \mathbb{Q}[[q]]. \end{aligned}$$

In the first chapter, we saw that these series, by setting $q = \exp(2\pi i\tau)$, appear in the Fourier expansion of the multiple Eisenstein series but in this section we just view them as formal power series. We refer to these generating functions of multiple divisor sums as *brackets* and define the vector space \mathcal{MD} to be the \mathbb{Q} vector space generated by $1 \in \mathbb{Q}[[q]]$

¹Further, one can prove the relation $\zeta(3) = \zeta(2, 1)$ between multiple zeta values by multiplying both sides in (2.3) with $(1 - q)^3$ and then take the limit $q \rightarrow 1$. We will discuss this in Chapter 5

and all brackets $[s_1, \dots, s_l]$. It is important to notice that we also include the constants in the space \mathcal{MD} .

Example 2.1. We give a few examples:

$$\begin{aligned} [2] &= q + 3q^2 + 4q^3 + 7q^4 + 6q^5 + 12q^6 + 8q^7 + 15q^8 + \dots, \\ [4, 2] &= \frac{1}{6} (q^3 + 3q^4 + 15q^5 + 27q^6 + 78q^7 + 135q^8 + \dots), \\ [4, 4, 4] &= \frac{1}{216} (q^6 + 9q^7 + 45q^8 + 190q^9 + 642q^{10} + 1899q^{11} + \dots), \\ [3, 1, 3, 1] &= \frac{1}{4} (q^{10} + 2q^{11} + 8q^{12} + 16q^{13} + 43q^{14} + 70q^{15} + \dots), \\ [1, 2, 3, 4, 5] &= \frac{1}{288} (q^{15} + 17q^{16} + 107q^{17} + 512q^{18} + 1985q^{19} + \dots). \end{aligned}$$

Notice that the first non vanishing coefficient of q^n in $[s_1, \dots, s_l]$ appears at $n = \frac{l(l+1)}{2}$, because it belongs to the "smallest" possible partition

$$l \cdot 1 + (l-1) \cdot 1 + \dots + 1 \cdot 1 = n,$$

i.e. $u_j = j$ and $v_j = 1$ for $1 \leq j \leq l$. The number $k = s_1 + \dots + s_l$ is called the *weight* of $[s_1, \dots, s_l]$ and l denotes the *length*.

We want to show that the brackets are closed under multiplication by proving that their product structure is an example for a quasi-shuffle product. To do this we first introduce some notations and quote some results which are needed for this.

Recall that for $s, z \in \mathbb{C}$, $|z| < 1$ the polylogarithm $\text{Li}_s(z)$ of weight s is given by $\text{Li}_s(z) = \sum_{n>0} \frac{z^n}{n^s}$. For $s \in \mathbb{N}$ the $\text{Li}_{-s}(z)$ are rational functions in z with a pole in $z = 1$. More precisely for $|z| < 1$ they can be written as

$$\text{Li}_{-s}(z) = \sum_{n>0} n^s z^n = \frac{z P_s(z)}{(1-z)^{s+1}}$$

where $P_s(z)$ is the s -th Eulerian polynomial. Such a polynomial is given by

$$P_s(X) = \sum_{n=0}^{s-1} A_{s,n} X^n,$$

where the Eulerian numbers $A_{s,n}$ are defined by

$$A_{s,n} = \sum_{i=0}^n (-1)^i \binom{s+1}{i} (n+1-i)^s.$$

For our purpose we write

$$\widetilde{\text{Li}}_{1-s}(z) := \frac{\text{Li}_{1-s}(z)}{(s-1)!}.$$

Lemma 2.2. ([BK, Lemma 2.5]) For $s_1, \dots, s_l \in \mathbb{N}$ we have

$$\begin{aligned} [s_1, \dots, s_l] &= \sum_{n_1 > \dots > n_l > 0} \widetilde{\text{Li}}_{1-s_1}(q^{n_1}) \dots \widetilde{\text{Li}}_{1-s_l}(q^{n_l}) \\ &= \frac{1}{(s_1-1)! \dots (s_l-1)!} \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{q^{n_j} P_{s_j-1}(q^{n_j})}{(1-q^{n_j})^{s_j}}. \end{aligned}$$

□

Remark 2.3. i) The second expression in terms of Eulerian Polynomials will be important for the interpretation of these series as q -analogues of multiple zeta values in Chapter 5.

ii) This representation is also used for a fast implementation of these q -series in Pari GP. By doing so, the authors in [BK] were able to give various results on the dimensions of the (weight and length filtered) spaces of \mathcal{MD} . These results can be found in Section 5 of [BK].

The product of $[s_1]$ and $[s_2]$ can thus be written as

$$\begin{aligned} [s_1] \cdot [s_2] &= \sum_{n_1 > n_2 > 0} \widetilde{\text{Li}}_{1-s_1}(q^{n_1}) \widetilde{\text{Li}}_{1-s_2}(q^{n_2}) + \sum_{n_2 > n_1 > 0} \dots + \sum_{n_1 = n_2 > 0} \widetilde{\text{Li}}_{1-s_1}(q^{n_1}) \widetilde{\text{Li}}_{1-s_2}(q^{n_1}) \\ &= [s_1, s_2] + [s_2, s_1] + \sum_{n > 0} \widetilde{\text{Li}}_{1-s_1}(q^n) \widetilde{\text{Li}}_{1-s_2}(q^n). \end{aligned}$$

In order to prove that this product is an element of \mathcal{MD} the product $\widetilde{\text{Li}}_{1-s_1}(q^n) \widetilde{\text{Li}}_{1-s_2}(q^n)$ must be a rational linear combination of $\widetilde{\text{Li}}_{1-j}(q^n)$ with $1 \leq j \leq s_1 + s_2$. We therefore need the following

Lemma 2.4. For $a, b \in \mathbb{N}$ we have

$$\widetilde{\text{Li}}_{1-a}(z) \cdot \widetilde{\text{Li}}_{1-b}(z) = \sum_{j=1}^a \lambda_{a,b}^j \widetilde{\text{Li}}_{1-j}(z) + \sum_{j=1}^b \lambda_{b,a}^j \widetilde{\text{Li}}_{1-j}(z) + \widetilde{\text{Li}}_{1-(a+b)}(z),$$

where the coefficient $\lambda_{a,b}^j \in \mathbb{Q}$ for $1 \leq j \leq a$ is given by

$$\lambda_{a,b}^j = (-1)^{b-1} \binom{a+b-j-1}{a-j} \frac{B_{a+b-j}}{(a+b-j)!},$$

with B_k being the k -th Bernoulli number¹

¹For convenience we recall that the Bernoulli numbers B_k are defined by $\frac{x}{e^x-1} =: \sum_{k \geq 0} \frac{B_k}{k!} X^k$.

Proof. We prove this by using the generating function

$$L(X) := \sum_{k>0} \widetilde{\text{Li}}_{1-k}(z) X^{k-1} = \sum_{k>0} \sum_{n>0} \frac{n^{k-1} z^n}{(k-1)!} X^{k-1} = \sum_{n>0} e^{nX} z^n = \frac{e^X z}{1 - e^X z}.$$

With this one can see by direct calculation that

$$L(X) \cdot L(Y) = \frac{1}{e^{X-Y} - 1} L(X) + \frac{1}{e^{Y-X} - 1} L(Y).$$

By the definition of the Bernoulli numbers

$$\frac{X}{e^X - 1} = \sum_{n \geq 0} \frac{B_n}{n!} X^n$$

this can be written as

$$L(X) \cdot L(Y) = \sum_{n>0} \frac{B_n}{n!} (X - Y)^{n-1} L(X) + \sum_{n>0} \frac{B_n}{n!} (Y - X)^{n-1} L(Y) + \frac{L(X) - L(Y)}{X - Y}.$$

The statement then follows by calculating the coefficient of $X^{a-1} Y^{b-1}$ in this equation. \square

Now we are able to interpret the product structure of brackets as an example for a quasi-shuffle product. We equip \mathfrak{H}^1 with a third product, beside the stuffle product $*$ and the shuffle product \sqcup . This product will be denoted \boxtimes , since it can be seen as a "bracket version" of the stuffle product $*$. For $a, b \in \mathbb{N}$ and $w, v \in \mathfrak{H}^1$ we define recursively the product

$$z_a w \boxtimes z_b v = z_a (w \boxtimes z_b v) + z_b (z_a w \boxtimes v) + z_{a+b} (w \boxtimes v) + \sum_{j=1}^a \lambda_{a,b}^j z_j (w \boxtimes v) + \sum_{j=1}^b \lambda_{b,a}^j z_j (w \boxtimes v),$$

where the coefficients $\lambda_{a,b}^j \in \mathbb{Q}$ are the same as in Lemma 2.5. We equip \mathcal{MD} with the usual multiplication of formal q -series and obtain the following:

Theorem 2.5. ([BK, Prop 2.10]) For the linear map $[\cdot] : (\mathfrak{H}^1, \boxtimes) \longrightarrow (\mathcal{MD}, \cdot)$ defined on the generators $w = z_{s_1} \dots z_{s_l}$ by $[w] := [s_1, \dots, s_l]$ we have

$$[w \boxtimes v] = [w] \cdot [v]$$

and therefore \mathcal{MD} is a \mathbb{Q} -algebra and $[\cdot]$ an algebra homomorphism. \square

Example 2.6. The first products of brackets are given by

$$\begin{aligned}
 [1] \cdot [1] &= 2[1, 1] + [2] - [1], \\
 [1] \cdot [2] &= [1, 2] + [2, 1] + [3] - \frac{1}{2}[2], \\
 [1] \cdot [2, 1] &= [1, 2, 1] + 2[2, 1, 1] - \frac{3}{2}[2, 1] + [2, 2] + [3, 1], \\
 [2] \cdot [3] &= [3, 2] + [2, 3] + [5] - \frac{1}{12}[3], \\
 [3] \cdot [2, 1] &= [3, 2, 1] + [2, 3, 1] + [2, 1, 3] + [5, 1] + [2, 4] + \frac{1}{12}[2, 2] - \frac{1}{2}[2, 3] - \frac{1}{12}[3, 1].
 \end{aligned}$$

We end this section by some notations which are needed for the rest of this thesis.

Definition 2.3. On \mathcal{MD} we have the increasing filtration $\text{Fil}_\bullet^{\text{W}}$ given by the weight and the increasing filtration $\text{Fil}_\bullet^{\text{L}}$ given by the length. For a subset $A \subset \mathcal{MD}$ we write

$$\begin{aligned}
 \text{Fil}_k^{\text{W}}(A) &:= \langle [s_1, \dots, s_l] \in A \mid s_1 + \dots + s_l \leq k \rangle_{\mathbb{Q}}, \\
 \text{Fil}_l^{\text{L}}(A) &:= \langle [s_1, \dots, s_r] \in A \mid r \leq l \rangle_{\mathbb{Q}}.
 \end{aligned}$$

If we consider the length and weight filtration at the same time, we use the short notation $\text{Fil}_{k,l}^{\text{W,L}} := \text{Fil}_k^{\text{W}} \text{Fil}_l^{\text{L}}$.

Remark 2.7. As it can be seen by Theorem 2.6, the multiplication of two brackets respects these filtrations, i.e.

$$\text{Fil}_{k_1,l_1}^{\text{W,L}}(\mathcal{MD}) \cdot \text{Fil}_{k_2,l_2}^{\text{W,L}}(\mathcal{MD}) \subset \text{Fil}_{k_1+k_2,l_1+l_2}^{\text{W,L}}(\mathcal{MD}).$$

2.4 Derivatives and Subalgebras

In this section we want to give an overview of interesting subalgebras of the space \mathcal{MD} and discuss the differential structure with respect to the differential $d = q \frac{d}{dq}$. One of the main results in [BK] is the following

Theorem 2.8. ([BK, Thm. 1.7]) The operator $d = q \frac{d}{dq}$ is a derivation on \mathcal{MD} , it maps $\text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD})$ to $\text{Fil}_{k+2,l+1}^{\text{W,L}}(\mathcal{MD})$. \square

The proof of Theorem 2.10 uses generating functions of the brackets. It gives explicit formulas for the derivatives $d[s_1, \dots, s_l]$ for all l which we omit here, since they are com-

plicated. For example we have

$$\begin{aligned} d[2, 1, 1] &= -\frac{1}{6}[2, 1, 1] + \frac{1}{2}[2, 1, 2] - [2, 1, 2, 1] + [2, 1, 3] + \frac{3}{2}[2, 2, 1] \\ &\quad - 2[2, 2, 1, 1] + [2, 3, 1] + 6[3, 1, 1] - 8[3, 1, 1, 1] + [4, 1, 1]. \end{aligned}$$

In the following we give a list of subalgebras and review the results on whether they are also closed under d or not.

i) (quasi-)modular forms: Next to the connection to modular forms due to their appearance in the Fourier expansion of multiple Eisenstein series, the brackets have a direct connection to quasi-modular forms for $SL_2(\mathbb{Z})$ with rational coefficients. In the case $l = 1$ we get the divisor sums $\sigma_{k-1}(n) = \sum_{d|n} d^{k-1}$ and

$$[k] = \frac{1}{(k-1)!} \sum_{n>0} \sigma_{k-1}(n) q^n.$$

These simple brackets appear in the Fourier expansion of classical Eisenstein series with rational coefficients $\tilde{G}_k(\tau) := (-2\pi i)^{-k} G_k(\tau)$ since we also included the rational numbers in \mathcal{MD} . For example we have

$$\tilde{G}_2 = -\frac{1}{24} + [2], \quad \tilde{G}_4 = \frac{1}{1440} + [4], \quad \tilde{G}_6 = -\frac{1}{60480} + [6].$$

Denote by $M_{\mathbb{Q}}(SL_2(\mathbb{Z})) = \mathbb{Q}[G_4, G_6]$ and $\tilde{M}_{\mathbb{Q}}(SL_2(\mathbb{Z})) = \mathbb{Q}[G_2, G_4, G_6]$ the algebras of modular forms and quasi-modular forms with rational coefficients.

It is a well-known fact that the space $\tilde{M}_{\mathbb{Q}}(SL_2(\mathbb{Z}))$ is closed under the operator $d = q \frac{d}{dq}$.

ii) Admissible brackets: We define the set of all admissible brackets $q\mathcal{MZ}$ as the span of all brackets $[s_1, \dots, s_l]$ with $s_1 > 1$ and 1. This space is a subalgebra of \mathcal{MD} ([BK, Thm. 2.13]) and every bracket can be written as a polynomial in the bracket $[1]$ with coefficients in $q\mathcal{MZ}$:

Theorem 2.9. ([BK, Thm. 2.14, Prop. 3.14])

- i) We have $\mathcal{MD} = q\mathcal{MZ}[[1]]$.
- ii) The algebra \mathcal{MD} is a polynomial ring over $q\mathcal{MZ}$ with indeterminate $[1]$, i.e. \mathcal{MD} is isomorphic to $q\mathcal{MZ}[T]$ by sending $[1]$ to T .
- iii) The space $q\mathcal{MZ}$ is closed under d . □

The elements in ${}_q\mathcal{MZ}$ are the ones, where the corresponding multiple zeta values exist. It will be reviewed in more detail in Chapter 5, when we consider the brackets as q -analogues of multiple zeta values.

iii) Even brackets and brackets with no 1's: Denote by $\mathcal{MD}^{\text{even}}$ the space spanned by 1 and all $[s_1, \dots, s_l]$ with s_j even for all $0 \leq j \leq l$ and by $\mathcal{MD}^\#$ the space spanned by 1 and all $[s_1, \dots, s_l]$ with $s_j > 1$. Both spaces $\mathcal{MD}^{\text{even}}$ and $\mathcal{MD}^\#$ are subalgebras of \mathcal{MD} ([BK, Prop. 2.15]). It is expected, that the space $\mathcal{MD}^{\text{even}}$ is not closed under d , since numerical calculation suggest, that for example $d[4, 2] \notin \mathcal{MD}^{\text{even}}$. Whether the space $\mathcal{MD}^\#$ is closed under this operator is an open and interesting question. In [BK2] it is shown, that this is actually equivalent to one part of Conjecture 1 in [O] given by Okounkov.

To summarize, we have the following inclusion of \mathbb{Q} -algebras

$$\begin{array}{ccccccc}
 & & \begin{array}{c} \text{d} \\ \curvearrowright \end{array} & & \begin{array}{c} \text{d?} \\ \curvearrowright \end{array} & & \begin{array}{c} \text{d} \\ \curvearrowright \end{array} & & \begin{array}{c} \text{d} \\ \curvearrowright \end{array} \\
 M_{\mathbb{Q}}(SL_2(\mathbb{Z})) & \hookrightarrow & \widetilde{M}_{\mathbb{Q}}(SL_2(\mathbb{Z})) & \hookrightarrow & \mathcal{MD}^{ev} & \hookrightarrow & \mathcal{MD}^\# & \hookrightarrow & {}_q\mathcal{MZ} & \hookrightarrow & \mathcal{MD} \\
 & & \begin{array}{c} \text{d} \\ \curvearrowleft \end{array} & & \begin{array}{c} \text{d?} \\ \curvearrowleft \end{array} & & & & & &
 \end{array}$$

The dashed arrows indicate the conjectured behavior of the map d , whereas the other arrows are all known to be correct.

Though in length $l = 1$ we derive not just one but several expressions for $d[s]$ given by the following Proposition.

Proposition 2.10. ([BK, Prop 3.3]) For s_1, s_2 with $s_1 + s_2 > 2$ and $s = s_1 + s_2 - 2$ we have the following expression for $d[s]$:

$$\binom{s}{s_1 - 1} \frac{d[s]}{s} = [s_1] \cdot [s_2] + \binom{s}{s_1 - 1} [s + 1] - \sum_{a+b=s+2} \left(\binom{a-1}{s_1 - 1} + \binom{a-1}{s_2 - 1} \right) [a, b].$$

If you compare this formula with the shuffle product of multiple zeta values (1.1) in the length one times length one case you notice that Proposition 2.12 basically states that the brackets fulfill the shuffle product up to the term $\binom{s}{s_1 - 1} \frac{d[s]}{s} - \binom{s}{s_1 - 1} [s + 1]$.

We end this chapter by using these formulas to prove the following identity

Proposition 2.11. The unique normalized cusp form Δ in weight 12 can be written as

$$\begin{aligned}
 -\frac{1}{2^6 \cdot 5 \cdot 691} \Delta &= 168[5, 7] + 150[7, 5] + 28[9, 3] \\
 &+ \frac{1}{1408}[2] - \frac{83}{14400}[4] + \frac{187}{6048}[6] - \frac{7}{120}[8] - \frac{5197}{691}[12].
 \end{aligned}$$

Proof. With the Eisenstein series \tilde{G}_6 and \tilde{G}_{12} given by

$$\begin{aligned}\tilde{G}_6 &= (-2\pi i)^{-6}\zeta(6) + [6] = -\frac{1}{60480} + [6], \\ \tilde{G}_{12} &= (-2\pi i)^{-12}\zeta(12) + [12] = \frac{691}{2615348736000} + [12],\end{aligned}$$

the cusp form Δ can be written as $\Delta = -3316800G_6^2 + 3432000G_{12}$. Using quasi-shuffle product of brackets one can derive

$$\Delta = \frac{3455}{198}[2] - \frac{691}{6}[4] + \frac{6910}{21}[6] + 115200[12] - 6633600[6, 6].$$

and therefore

$$-\frac{1}{2^6 \cdot 5 \cdot 691}\Delta = 30[6, 6] - \frac{1}{12672}[2] + \frac{1}{1920}[4] - \frac{1}{672}[6] - \frac{360}{691}[12]. \quad (2.4)$$

Using Proposition 2.12 for $(s_1, s_2) = (4, 8), (5, 7), (6, 6)$ we get the following three expressions for $d[10]$

$$\begin{aligned}d[10] &= -\frac{1}{3}[5, 7] - \frac{5}{6}[6, 6] - \frac{5}{3}[7, 5] - \frac{35}{12}[8, 4] - \frac{16}{3}[9, 3] - 10[10, 2] - 20[11, 1] \\ &\quad - \frac{1}{4790016}[2] + \frac{1}{403200}[4] - \frac{1}{36288}[6] + \frac{1}{8640}[8] + 10[11] + \frac{1}{12}[12], \\ d[10] &= -\frac{5}{21}[6, 6] - \frac{5}{7}[7, 5] - 2[8, 4] - \frac{14}{3}[9, 3] - 10[10, 2] - 20[11, 1] \\ &\quad + \frac{1}{4790016}[2] - \frac{1}{604800}[4] + \frac{1}{127008}[6] + 10[11] + \frac{1}{21}[12], \\ d[10] &= -\frac{10}{21}[7, 5] - \frac{5}{3}[8, 4] - \frac{40}{9}[9, 3] - 10[10, 2] - 20[11, 1] \\ &\quad - \frac{1}{4790016}[2] + \frac{1}{725760}[4] - \frac{1}{381024}[6] + 10[11] + \frac{5}{126}[12].\end{aligned}$$

Summing them up as $0 = -504 d[10] + 1890 d[10] - 1386 d[10]$ we get

$$\begin{aligned}0 &= 168[5, 7] - 30[6, 6] + 150[7, 5] + 28[9, 3] \\ &\quad + \frac{5}{6336}[2] - \frac{181}{28800}[4] + \frac{7}{216}[6] - \frac{7}{120}[8] - 7[12]\end{aligned} \quad (2.5)$$

Combining (2.5) and (2.4), in order to eliminate the occurrence of $[6, 6]$, we obtain the desired identity. \square

Chapter 3

Bi-brackets and a second product expression for brackets

In the previous chapter we have seen that the space \mathcal{MD} of brackets has the structure of a \mathbb{Q} -algebra and that there is an explicit formula to express the product of two brackets as a linear combination of brackets similarly to the stuffle product of multiple zeta values. In this chapter we want to present a larger class of q -series, called bi-brackets. The quasi-shuffle product of brackets extend to this larger class and therefore the space of bi-brackets is also a \mathbb{Q} -algebra. The beautiful feature of bi-brackets is, that there is a relation, which we call partition relation, which enables one to express the product of two bi-brackets in a second different way. These two product expressions then give a large class of linear relations, similar to the double shuffle relations of multiple zeta values. A variation of the bi-brackets were also studied in [Zu]. Later, the bi-brackets will be used to define regularized multiple Eisenstein series in Chapter 4. All results in this chapter were studied and introduced in [Ba2].

3.1 Bi-brackets and their generating series

As motivated in the introduction of this section we want to study the following q -series:

Definition 3.2. For $r_1, \dots, r_l \geq 0$, $s_1, \dots, s_l > 0$ and we define the following q -series

$$\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} := \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \frac{u_1^{r_1}}{r_1!} \cdots \frac{u_l^{r_l}}{r_l!} \cdot \frac{v_1^{s_1-1} \cdots v_l^{s_l-1}}{(s_1-1)! \cdots (s_l-1)!} \cdot q^{u_1 v_1 + \dots + u_l v_l} \in \mathbb{Q}[[q]]$$

which we call *bi-brackets* of weight $r_1 + \cdots + r_k + s_1 + \cdots + s_l$, upper weight $s_1 + \cdots + s_l$, lower weight $r_1 + \cdots + r_l$ and length l . By \mathcal{BD} we denote the \mathbb{Q} -vector space spanned by all bi-brackets and 1.

The factorial factors in the definition of bi-brackets will become natural when considering generating functions of bi-brackets and the connection to multiple zeta values.

For $r_1 = \cdots = r_l = 0$ the bi-brackets are just the brackets

$$\begin{bmatrix} s_1, \dots, s_l \\ 0, \dots, 0 \end{bmatrix} = [s_1, \dots, s_l]$$

as defined in Chapter 2. Similarly to the Definition 2.8 of the filtration for the space \mathcal{BD} we write for a subset $A \in \mathcal{BD}$

$$\begin{aligned} \text{Fil}_k^{\text{W}}(A) &:= \left\langle \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \in A \mid 0 \leq l \leq k, s_1 + \cdots + s_l \leq k \right\rangle_{\mathbb{Q}} \\ \text{Fil}_k^{\text{D}}(A) &:= \left\langle \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \in A \mid 0 \leq l \leq k, r_1 + \cdots + r_l \leq k \right\rangle_{\mathbb{Q}} \\ \text{Fil}_l^{\text{L}}(A) &:= \left\langle \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \in A \mid l \leq l \right\rangle_{\mathbb{Q}}. \end{aligned}$$

and again if we consider the length and weight filtration at the same time we use the short notation $\text{Fil}_{k,l}^{\text{W,L}} := \text{Fil}_k^{\text{W}} \text{Fil}_l^{\text{L}}$ and similar for the other filtrations.

Proposition 3.1. ([Ba2, Prop 4.2]) Let $d := q \frac{d}{dq}$, then we have

$$d \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} = \sum_{j=1}^l \left(s_j (r_j + 1) \begin{bmatrix} s_1, \dots, s_{j-1}, s_j + 1, s_{j+1}, \dots, s_l \\ r_1, \dots, r_{j-1}, r_j + 1, r_{j+1}, \dots, r_l \end{bmatrix} \right)$$

and therefore $d \left(\text{Fil}_{k,d,l}^{\text{W,D,L}}(\mathcal{BD}) \right) \subset \text{Fil}_{k+1,d+1,l}^{\text{W,D,L}}(\mathcal{BD})$.

Proof. This is an easy consequence of the definition of bi-brackets and the fact that $d \sum_{n>0} a_n q^n = \sum_{n>0} n a_n q^n$. □

Proposition 3.2 suggests that the bi-brackets can be somehow viewed as partial derivatives of the brackets with total differential d .

In the following we now want to discuss the algebra structure of the space \mathcal{BD} . For this we extend the quasi-shuffle product \boxtimes of \mathfrak{H}^1 to a larger space of words. Since we have double indices we replace the alphabet $A_z = \{z_1, z_2, \dots\}$ by $A_z^{\text{bi}} := \{z_{s,r} \mid s \geq 1, r \geq 0\}$.

We consider on $\mathbb{Q}A_z^{\text{bi}}$ the commutative and associative product

$$\begin{aligned} z_{s_1, r_1} \boxtimes z_{s_2, r_2} &= \binom{r_1 + r_2}{r_1} \sum_{j=1}^{s_1} \lambda_{s_1, s_2}^j z_{j, r_1 + r_2} + \binom{r_1 + r_2}{r_1} \sum_{j=1}^{s_2} \lambda_{s_2, s_1}^j z_{j, r_1 + r_2} \\ &\quad + \binom{r_1 + r_2}{r_1} z_{s_1 + s_2, r_1 + r_2} \end{aligned}$$

and on $\mathbb{Q}\langle A_z^{\text{bi}} \rangle$ the commutative and associative quasi-shuffle product

$$z_{s_1, r_1} w \boxtimes z_{s_2, r_2} v = z_{s_1, r_1} (w \boxtimes z_{s_2, r_2} v) + z_{s_2, r_2} (z_{s_1, r_1} w \boxtimes v) + (z_{s_1, r_1} \boxtimes z_{s_2, r_2})(w \boxtimes v),$$

where the the numbers $\lambda_{a,b}^j \in \mathbb{Q}$ for $1 \leq j \leq a$ are the same as before, i.e.

$$\lambda_{a,b}^j = (-1)^{b-1} \binom{a+b-j-1}{a-j} \frac{B_{a+b-j}}{(a+b-j)!}.$$

Theorem 3.2. ([Ba2, Thm. 3.6]) The map $[\cdot] : (\mathbb{Q}\langle A_z^{\text{bi}} \rangle, \boxtimes) \rightarrow (\mathcal{BD}, \cdot)$ given by

$$w = z_{s_1, r_1} \dots z_{s_l, r_l} \longmapsto [w] = \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix}$$

fulfills $[w \boxtimes v] = [w] \cdot [v]$ and therefore \mathcal{BD} is a \mathbb{Q} -algebra.

Definition 3.3. For the generating function of the bi-brackets we write

$$\left| \begin{array}{c} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{array} \right| := \sum_{\substack{s_1, \dots, s_l > 0 \\ r_1, \dots, r_l > 0}} \begin{bmatrix} s_1, \dots, s_l \\ r_1 - 1, \dots, r_l - 1 \end{bmatrix} X_1^{s_1-1} \dots X_l^{s_l-1} \cdot Y_1^{r_1-1} \dots Y_l^{r_l-1}.$$

These are elements in the ring $\mathcal{BD}_{\text{gen}} = \varinjlim_j \mathcal{BD}[[X_1, \dots, X_j, Y_1, \dots, Y_j]]$ of all generating series of bi-brackets.

To derive relations between bi-brackets we will prove functional equations for their generating functions. The key fact for this is that there are two different ways of expressing these given by the following Theorem.

Theorem 3.3. ([Ba2, Thm. 2.3]) For $n \in \mathbb{N}$ set

$$E_n(X) := e^{nX} \quad \text{and} \quad L_n(X) := \frac{e^X q^n}{1 - e^X q^n} \in \mathbb{Q}[[q, X]].$$

Then for all $l \geq 1$ we have the following two different expressions for the generating functions:

$$\begin{aligned} \left| \begin{array}{c} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{array} \right| &= \sum_{u_1 > \dots > u_l > 0} \prod_{j=1}^l E_{u_j}(Y_j) L_{u_j}(X_j) \\ &= \sum_{u_1 > \dots > u_l > 0} \prod_{j=1}^l E_{u_j}(X_{l+1-j} - X_{l+2-j}) L_{u_j}(Y_1 + \dots + Y_{l-j+1}) \end{aligned}$$

(with $X_{l+1} := 0$). In particular the *partition relations*¹ holds:

$$\left| \begin{array}{c} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{array} \right| \stackrel{P}{=} \left| \begin{array}{c} Y_1 + \dots + Y_l, \dots, Y_1 + Y_2, Y_1 \\ X_l, X_{l-1} - X_l, \dots, X_1 - X_2 \end{array} \right|. \quad (3.1)$$

□

Remark 3.4. A nice combinatorial explanation for the partition relation (3.1) is the following: By a partition of a natural number n with l parts we denote a representation of n as a sum of l distinct natural numbers, i.e. $15 = 4 + 4 + 3 + 2 + 1 + 1$ is a partition of 15 with the 4 parts given by 4, 3, 2, 1. We identify such a partition with a tuple $(u, v) \in \mathbb{N}^l \times \mathbb{N}^l$ where the u_j 's are the l distinct numbers in the partition and the v_j 's count their appearance in the sum. The above partition of 15 is therefore given by the tuple $(u, v) = ((4, 3, 2, 1), (2, 1, 1, 2))$. By $P_l(n)$ we denote all partitions of n with l parts and hence we set

$$P_l(n) := \left\{ (u, v) \in \mathbb{N}^l \times \mathbb{N}^l \mid n = u_1 v_1 + \dots + u_l v_l \text{ and } u_1 > \dots > u_l > 0 \right\}$$

On the set $P_l(n)$ one has an involution given by the conjugation ρ of partitions which can be obtained by reflecting the corresponding Young diagram across the main diagonal.

$$((4, 3, 2, 1), (2, 1, 1, 2)) = \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \\ \hline \square & \square & \square & \\ \hline \square & \square & & \\ \hline \square & & & \\ \hline \end{array} \xrightarrow{\rho} \begin{array}{|c|c|c|c|c|} \hline \square & \square & \square & \square & \square \\ \hline \square & \square & \square & \square & \\ \hline \square & \square & \square & \square & \\ \hline \square & \square & \square & & \\ \hline \square & \square & & & \\ \hline \square & & & & \\ \hline \end{array} = ((6, 4, 3, 2), (1, 1, 1, 1))$$

Figure 3.1: The conjugation of the partition $15 = 4 + 4 + 3 + 2 + 1 + 1$ is given by $\rho(((4, 3, 2, 1), (2, 1, 1, 2))) = ((6, 4, 3, 2), (1, 1, 1, 1))$ which can be seen by reflection the corresponding Young diagram at the main diagonal.

¹The bi-brackets and their generating series also give examples of what is called a *bimould* by Ecalle in [E]. In his language the partition relation (3.1) states that the bimould of generating series of bi-brackets is swap invariant.

On the set $P_l(n)$ the conjugation ρ is explicitly given by $\rho((u, v)) = (u', v')$ where $u'_j = v_1 + \cdots + v_{l-j+1}$ and $v'_j = u_{l-j+1} - u_{l-j+2}$ with $u_{l+1} := 0$, i.e.

$$\rho : \left(\begin{array}{c} u_1, \dots, u_l \\ v_1, \dots, v_l \end{array} \right) \mapsto \left(\begin{array}{c} v_1 + \cdots + v_l, \dots, v_1 + v_2, v_1 \\ u_l, u_{l-1} - u_l, \dots, u_1 - u_2 \end{array} \right). \quad (3.2)$$

By the definition of the bi-brackets its clear that with the above notation they can be written as

$$\left[\begin{array}{c} s_1, \dots, s_l \\ r_1, \dots, r_l \end{array} \right] := \frac{1}{r_1!(s_1-1)! \dots r_l!(s_l-1)!} \sum_{n>0} \left(\sum_{(u,v) \in P_l(n)} u_1^{r_1} v_1^{s_1-1} \dots u_l^{r_l} v_l^{s_l-1} \right) q^n.$$

The coefficients are given by a sum over all elements in $P_l(n)$ and therefore it is invariant under the action of ρ . As an example, consider $[2, 2]$ and apply ρ to the sum. Then we obtain

$$\begin{aligned} [2, 2] &= \sum_{n>0} \left(\sum_{(u,v) \in P_2(n)} v_1 \cdot v_2 \right) q^n = \sum_{n>0} \left(\sum_{\rho((u,v)) = (u',v') \in P_2(n)} u'_2 \cdot (u'_1 - u'_2) \right) q^n \\ &= \sum_{n>0} \left(\sum_{(u',v') \in P_2(n)} u'_2 \cdot u'_1 \right) q^n - \sum_{n>0} \left(\sum_{(u',v') \in P_2(n)} u'^2_2 \right) q^n = \begin{bmatrix} 1, 1 \\ 1, 1 \end{bmatrix} - 2 \begin{bmatrix} 1, 1 \\ 0, 2 \end{bmatrix}. \end{aligned} \quad (3.3)$$

This is exactly the relation one obtains by using the partition relation.

Corollary 3.5. (*[Ba2, Cor. 2.5]*) (*Partition relation in length one and two*) For $r, r_1, r_2 \geq 0$ and $s, s_1, s_2 > 0$ we have the following relations in length one and two

$$\begin{aligned} \begin{bmatrix} s \\ r \end{bmatrix} &= \begin{bmatrix} r+1 \\ s-1 \end{bmatrix}, \\ \begin{bmatrix} s_1, s_2 \\ r_1, r_2 \end{bmatrix} &= \sum_{\substack{0 \leq j \leq r_1 \\ 0 \leq k \leq s_2-1}} (-1)^k \binom{s_1-1+k}{k} \binom{r_2+j}{j} \begin{bmatrix} r_2+j+1, r_1-j+1 \\ s_2-1-k, s_1-1+k \end{bmatrix}. \end{aligned}$$

□

Remark 3.6. If we replace in the generating series in Definition 3.4 the bi-brackets by the corresponding bi-words in and enforce the partition relation (3.1) for this power series, we obtain an involution

$$P : \mathbb{Q}\langle A_z^{\text{bi}} \rangle \rightarrow \mathbb{Q}\langle A_z^{\text{bi}} \rangle.$$

By Corollary 3.7 it is for example $P(z_{s,r}) = z_{r+1, s-1}$. This will be needed to describe the second product structure in the next section.

3.4 Double shuffle relations for bi-brackets

The partition relation together with the quasi-shuffle product can be used to obtain a second expression for the product of two bi-brackets. Before giving the general explanation this second product expression we illustrate it in two examples.

Example 3.7. i) We want to give a second product expression for the product $[2] \cdot [3]$. By the partition relation we know that $[2] = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $[3] = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ and using the quasi-shuffle product we have

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 1, 1 \\ 1, 2 \end{bmatrix} + \begin{bmatrix} 1, 1 \\ 2, 1 \end{bmatrix} - 3 \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 3 \begin{bmatrix} 2 \\ 3 \end{bmatrix}.$$

The partition relations for the length two bi-brackets on the right is given by

$$\begin{aligned} \begin{bmatrix} 1, 1 \\ 1, 2 \end{bmatrix} &= \begin{bmatrix} 3, 2 \\ 0, 0 \end{bmatrix} + 3 \begin{bmatrix} 4, 1 \\ 0, 0 \end{bmatrix} = [3, 2] + 3[4, 1], \\ \begin{bmatrix} 1, 1 \\ 2, 1 \end{bmatrix} &= \begin{bmatrix} 2, 3 \\ 0, 0 \end{bmatrix} + 2 \begin{bmatrix} 3, 2 \\ 0, 0 \end{bmatrix} + 3 \begin{bmatrix} 4, 1 \\ 0, 0 \end{bmatrix} = [2, 3] + 2[3, 2] + 3[4, 1]. \end{aligned}$$

Combining all of this we obtain

$$\begin{aligned} \begin{bmatrix} 2 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 0 \end{bmatrix} &= \begin{bmatrix} 1 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 2 \end{bmatrix} \\ &= \begin{bmatrix} 1, 1 \\ 1, 2 \end{bmatrix} + \begin{bmatrix} 1, 1 \\ 2, 1 \end{bmatrix} - 3 \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 3 \begin{bmatrix} 2 \\ 3 \end{bmatrix} \\ &= [2, 3] + 3[3, 2] + 6[4, 1] + 3 \begin{bmatrix} 4 \\ 1 \end{bmatrix} - 3[4]. \end{aligned}$$

Compare this to the shuffle product of multiple zeta values

$$\zeta(2)\zeta(3) = \zeta(2, 3) + 3\zeta(3, 2) + 6\zeta(4, 1).$$

Since $d[3] = 3 \begin{bmatrix} 4 \\ 1 \end{bmatrix}$ this example exactly coincides with the formula in Proposition 2.12 for the derivative $d[k]$.

- ii) In higher length, expressing the product of two bi-brackets in a similar way as in i) becomes interesting, since then the extra terms can't be expressed with the operator d

anymore. Doing the same calculation for the product $[3] \cdot [2, 1]$, i.e. using the partition relation, the quasi-shuffle product and again the partition relation we obtain

$$\begin{aligned}
 [3] \cdot [2, 1] &= \begin{bmatrix} 1 \\ 2 \end{bmatrix} \cdot \begin{bmatrix} 1, 1 \\ 0, 1 \end{bmatrix} \\
 &= \begin{bmatrix} 1, 1, 1 \\ 2, 0, 1 \end{bmatrix} + \begin{bmatrix} 1, 1, 1 \\ 0, 2, 1 \end{bmatrix} + \begin{bmatrix} 1, 1, 1 \\ 0, 1, 2 \end{bmatrix} + 3 \begin{bmatrix} 1, 2 \\ 0, 3 \end{bmatrix} + \begin{bmatrix} 2, 1 \\ 2, 1 \end{bmatrix} - 3 \begin{bmatrix} 1, 1 \\ 0, 3 \end{bmatrix} - \begin{bmatrix} 1, 1 \\ 2, 1 \end{bmatrix} \\
 &= [2, 1, 3] + [2, 2, 2] + 2[2, 3, 1] + 2[3, 1, 2] + 5[3, 2, 1] + 9[4, 1, 1] \\
 &\quad + \begin{bmatrix} 2, 3 \\ 0, 1 \end{bmatrix} + 2 \begin{bmatrix} 3, 2 \\ 0, 1 \end{bmatrix} + 3 \begin{bmatrix} 4, 1 \\ 1, 0 \end{bmatrix} - [2, 3] - 2[3, 2] - 6[4, 1].
 \end{aligned}$$

This product can be seen as the analog of the shuffle product

$$\zeta(3) \cdot \zeta(2, 1) = \zeta(2, 1, 3) + \zeta(2, 2, 2) + 2\zeta(2, 3, 1) + 2\zeta(3, 1, 2) + 5\zeta(3, 2, 1) + 9\zeta(4, 1, 1).$$

Here the bi-brackets, which are not given as brackets, can not be written in terms of the operator d in an obvious way.

This works for arbitrary lengths and yields a natural way to obtain the second product expression for bi-brackets. To be more precise, denote by $P : \mathbb{Q}\langle A_z^{\text{bi}} \rangle \rightarrow \mathbb{Q}\langle A_z^{\text{bi}} \rangle$ the involution defined in Remark 3.8. Using this convention the second product expression for bi-brackets can be written in $\mathbb{Q}\langle A_z^{\text{bi}} \rangle$ for two words $u, v \in \mathbb{Q}\langle A_z^{\text{bi}} \rangle$ as $P(P(u) \boxtimes P(v))$, i.e. the two product expressions of bi-brackets which correspond to the stuffle and shuffle product of multiple zeta values are given by

$$[u] \cdot [v] = [u \boxtimes v], \quad [u] \cdot [v] = [P(P(u) \boxtimes P(v))]. \quad (3.4)$$

In contrast to multiple zeta values these two product expression are the same for some cases, as one can check for the example $[1] \cdot [1, 1]$. In the smallest length case, we have the following explicit formulas for the two products expressions.

Proposition 3.8. ([Ba, Prop. 3.3]) For $s_1, s_2 > 0$ and $r_1, r_2 \geq 0$ we have the following two expressions for the product of two bi-brackets of length one:

i) ("Stuffle product analog for bi-brackets")

$$\begin{aligned}
 \begin{bmatrix} s_1 \\ r_1 \end{bmatrix} \cdot \begin{bmatrix} s_2 \\ r_2 \end{bmatrix} &= \begin{bmatrix} s_1, s_2 \\ r_1, r_2 \end{bmatrix} + \begin{bmatrix} s_2, s_1 \\ r_2, r_1 \end{bmatrix} + \binom{r_1 + r_2}{r_1} \begin{bmatrix} s_1 + s_2 \\ r_1 + r_2 \end{bmatrix} \\
 &\quad + \binom{r_1 + r_2}{r_1} \sum_{j=1}^{s_1} \frac{(-1)^{s_2-1} B_{s_1+s_2-j}}{(s_1 + s_2 - j)!} \binom{s_1 + s_2 - j - 1}{s_1 - j} \begin{bmatrix} j \\ r_1 + r_2 \end{bmatrix} \\
 &\quad + \binom{r_1 + r_2}{r_1} \sum_{j=1}^{s_2} \frac{(-1)^{s_1-1} B_{s_1+s_2-j}}{(s_1 + s_2 - j)!} \binom{s_1 + s_2 - j - 1}{s_2 - j} \begin{bmatrix} j \\ r_1 + r_2 \end{bmatrix}
 \end{aligned}$$

ii) ("Shuffle product analog for bi-brackets")

$$\begin{aligned}
 \begin{bmatrix} s_1 \\ r_1 \end{bmatrix} \cdot \begin{bmatrix} s_2 \\ r_2 \end{bmatrix} &= \sum_{\substack{1 \leq j \leq s_1 \\ 0 \leq k \leq r_2}} \binom{s_1 + s_2 - j - 1}{s_1 - j} \binom{r_1 + r_2 - k}{r_1} (-1)^{r_2 - k} \begin{bmatrix} s_1 + s_2 - j, j \\ k, r_1 + r_2 - k \end{bmatrix} \\
 &+ \sum_{\substack{1 \leq j \leq s_2 \\ 0 \leq k \leq r_1}} \binom{s_1 + s_2 - j - 1}{s_1 - 1} \binom{r_1 + r_2 - k}{r_1 - k} (-1)^{r_1 - k} \begin{bmatrix} s_1 + s_2 - j, j \\ k, r_1 + r_2 - k \end{bmatrix} \\
 &+ \binom{s_1 + s_2 - 2}{s_1 - 1} \begin{bmatrix} s_1 + s_2 - 1 \\ r_1 + r_2 + 1 \end{bmatrix} \\
 &+ \binom{s_1 + s_2 - 2}{s_1 - 1} \sum_{j=0}^{r_1} \frac{(-1)^{r_2} B_{r_1 + r_2 - j + 1}}{(r_1 + r_2 - j + 1)!} \binom{r_1 + r_2 - j}{r_1 - j} \begin{bmatrix} s_1 + s_2 - 1 \\ j \end{bmatrix} \\
 &+ \binom{s_1 + s_2 - 2}{s_1 - 1} \sum_{j=0}^{r_2} \frac{(-1)^{r_1} B_{r_1 + r_2 - j + 1}}{(r_1 + r_2 - j + 1)!} \binom{r_1 + r_2 - j}{r_2 - j} \begin{bmatrix} s_1 + s_2 - 1 \\ j \end{bmatrix}
 \end{aligned}$$

Having these two expressions for the product of bi-brackets we obtain a large family of linear relations between them. Computer experiments suggest that actually every bi-bracket can be written in terms of brackets and that motivates the following surprising conjecture.

Conjecture 3.9. The algebra \mathcal{BD} of bi-brackets is a subalgebra of \mathcal{MD} and in particular we have

$$\text{Fil}_{k,d,l}^{\text{W,D,L}}(\mathcal{BD}) \subset \text{Fil}_{k+d,l+d}^{\text{W,L}}(\mathcal{MD}).$$

The results towards this conjecture, beside the computer experiments which have been done up to weight 8, are the following

Proposition 3.10. ([Ba2, Prop. 4.4]) For $l = 1$ the Conjecture 3.11 is true.

In [BK3] it will be shown, that Conjecture 3.11 is also true for all length up to weight 7. For higher weights and lengths there are no general statements. The only general statement for the length two case is given by the following Proposition.

Proposition 3.11. ([Ba2, Prop. 5.9]) For all $s_1, s_2 \geq 1$ it is

$$\begin{bmatrix} s_1, s_2 \\ 1, 0 \end{bmatrix}, \begin{bmatrix} s_1, s_2 \\ 0, 1 \end{bmatrix} \in \text{Fil}_{s_1 + s_2 + 1, 3}^{\text{W,L}}(\mathcal{MD})$$

□

3.5 The shuffle brackets

We now want to define a q -series which is an element in \mathcal{BD} and whose products can be written in terms of the "real" shuffle product of multiple zeta values. For $e_1, \dots, e_l \geq 1$ we generalize the generating function of bi-brackets to the following

$$\left| \begin{array}{c} X_1, \dots, X_l \\ Y_1, \dots, Y_l \\ e_1, \dots, e_l \end{array} \right| = \sum_{u_1 > \dots > u_l > 0} \prod_{j=1}^l E_{u_j}(Y_j) L_{u_j}(X_j)^{e_j}. \quad (3.5)$$

In particular for $e_1 = \dots = e_l = 1$ these are the generating functions of the bi-brackets. To show that the coefficients of these series are in \mathcal{BD} for arbitrary e_j we need to define the differential operator $\mathcal{D}_{e_1, \dots, e_l}^Y := D_{Y_1, e_1} D_{Y_2, e_2} \dots D_{Y_l, e_l}$ with

$$D_{Y_j, e} = \prod_{k=1}^{e-1} \left(\frac{1}{k} \left(\frac{\partial}{\partial Y_{l-j+1}} - \frac{\partial}{\partial Y_{l-j+2}} \right) - 1 \right).$$

where we set $\frac{\partial}{\partial Y_{l+1}} = 0$.

Lemma 3.12. Let \mathcal{A} be an algebra spanned by elements a_{s_1, \dots, s_l} with $s_1, \dots, s_l \in \mathbb{N}$, let $H(X_1, \dots, X_l) = \sum_{s_j} a_{s_1, \dots, s_l} X_1^{s_1-1} \dots X_l^{s_l-1}$ be the generating functions of these elements and define for $f \in \mathbb{Q}[[X_1, \dots, X_l]]$

$$f^\sharp(X_1, \dots, X_l) = f(X_1 + \dots + X_l, X_2 + \dots + X_l, \dots, X_l).$$

Then the following two statements are equivalent.

- i) The map $(\mathfrak{H}^1, \sqcup) \rightarrow \mathcal{A}$ given by $z_{s_1} \dots z_{s_l} \mapsto a_{s_1, \dots, s_l}$ is an algebra homomorphism.
- ii) For all $r, s \in \mathbb{N}$ it is

$$H^\sharp(X_1, \dots, X_r) \cdot H^\sharp(X_{r+1}, \dots, X_{r+s}) = H^\sharp(X_1, \dots, X_{r+s})_{|sh_r^{(r+s)}},$$

where $sh_r^{(r+s)} = \sum_{\sigma \in \Sigma(r,s)} \sigma$ in the group ring $\mathbb{Z}[\mathfrak{S}_{r+s}]$ and the symmetric group \mathfrak{S}_r acts on $\mathbb{Q}[[X_1, \dots, X_r]]$ by $(f|_\sigma)(X_1, \dots, X_r) = f(X_{\sigma^{-1}(1)}, \dots, X_{\sigma^{-1}(r)})$.

Proof. This can be proven by induction over l together with Proposition 8 in [I]. \square

Theorem 3.13. ([Ba2, Thm. 5.7]) For $s_1, \dots, s_l \in \mathbb{N}$ define $[s_1, \dots, s_l]^\sqcup \in \mathcal{BD}$ as the coefficients of the following generating function

$$\begin{aligned} H_\sqcup(X_1, \dots, X_l) &= \sum_{s_1, \dots, s_l \geq 1} [s_1, \dots, s_l]^\sqcup X_1^{s_1-1} \dots X_l^{s_l-1} \\ &:= \sum_{\substack{1 \leq m \leq l \\ i_1 + \dots + i_m = l}} \frac{1}{i_1! \dots i_m!} \mathcal{D}_{i_1, \dots, i_m}^Y \left| \begin{array}{c} X_1, X_{i_m+1}, X_{i_{m-1}+i_m+1}, \dots, X_{i_2+\dots+i_m+1} \\ Y_1, \dots, Y_l \end{array} \right|_{Y=0}. \end{aligned}$$

Then we have the following two statements

i) The $[s_1, \dots, s_l]^{\sqcup}$ fulfill the shuffle product, i.e.

$$H_{\sqcup}^{\sharp}(X_1, \dots, X_r) \cdot H_{\sqcup}^{\sharp}(X_{r+1}, \dots, X_{r+s}) = H_{\sqcup}^{\sharp}(X_1, \dots, X_{r+s})_{|sh_r^{(r+s)}}.$$

ii) For $s_1 \geq 1, s_2, \dots, s_l \geq 2$ we have $[s_1, \dots, s_l]^{\sqcup} = [s_1, \dots, s_l]$.

□

For low lengths we obtain the following examples:

Corollary 3.14. *It is $[s_1]^{\sqcup} = [s_1]$ and for $l = 2, 3, 4$ the $[s_1, \dots, s_l]^{\sqcup}$ are given by*

$$i) [s_1, s_2]^{\sqcup} = [s_1, s_2] + \delta_{s_2,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1 \\ 1 \end{bmatrix} - [s_1] \right),$$

$$ii) [s_1, s_2, s_3]^{\sqcup} = [s_1, s_2, s_3] + \delta_{s_3,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_2 \\ 0, 1 \end{bmatrix} - [s_1, s_2] \right) \\ + \delta_{s_2,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_3 \\ 1, 0 \end{bmatrix} - \begin{bmatrix} s_1, s_3 \\ 0, 1 \end{bmatrix} - [s_1, s_3] \right) \\ + \delta_{s_2 \cdot s_3, 1} \cdot \frac{1}{6} \left(\begin{bmatrix} s_1 \\ 2 \end{bmatrix} - \frac{3}{2} \begin{bmatrix} s_1 \\ 1 \end{bmatrix} + [s_1] \right),$$

$$iii) [s_1, s_2, s_3, s_4]^{\sqcup} = [s_1, s_2, s_3, s_4] + \delta_{s_4,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_2, s_3 \\ 0, 0, 1 \end{bmatrix} - [s_1, s_2, s_3] \right) \\ + \delta_{s_3,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_2, s_4 \\ 0, 1, 0 \end{bmatrix} - \begin{bmatrix} s_1, s_2, s_4 \\ 0, 0, 1 \end{bmatrix} + [s_1, s_2, s_4] \right) \\ + \delta_{s_2,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_3, s_4 \\ 1, 0, 0 \end{bmatrix} - \begin{bmatrix} s_1, s_3, s_4 \\ 0, 1, 0 \end{bmatrix} + [s_1, s_3, s_4] \right) \\ + \delta_{s_2 \cdot s_4, 1} \cdot \frac{1}{4} \left(\begin{bmatrix} s_1, s_3 \\ 1, 1 \end{bmatrix} - 2 \begin{bmatrix} s_1, s_3 \\ 0, 2 \end{bmatrix} - \begin{bmatrix} s_1, s_3 \\ 1, 0 \end{bmatrix} + [s_1, s_3] \right) \\ + \delta_{s_3 \cdot s_4, 1} \cdot \frac{1}{6} \left(\begin{bmatrix} s_1, s_2 \\ 0, 2 \end{bmatrix} - \frac{3}{2} \begin{bmatrix} s_1, s_2 \\ 0, 1 \end{bmatrix} + [s_1, s_2] \right) \\ + \delta_{s_2 \cdot s_3, 1} \cdot \frac{1}{6} \left(\begin{bmatrix} s_1, s_4 \\ 0, 2 \end{bmatrix} - \begin{bmatrix} s_1, s_4 \\ 1, 1 \end{bmatrix} + \frac{3}{2} \begin{bmatrix} s_1, s_4 \\ 0, 1 \end{bmatrix} + \begin{bmatrix} s_1, s_4 \\ 2, 0 \end{bmatrix} - \frac{3}{2} \begin{bmatrix} s_1, s_4 \\ 1, 0 \end{bmatrix} + [s_1, s_4] \right) \\ + \delta_{s_2 \cdot s_3 \cdot s_4, 1} \cdot \frac{1}{24} \left(\begin{bmatrix} s_1 \\ 3 \end{bmatrix} - 2 \begin{bmatrix} s_1 \\ 2 \end{bmatrix} + \frac{11}{6} \begin{bmatrix} s_1 \\ 1 \end{bmatrix} - [s_1] \right).$$

Proof. This follows by calculating the coefficients of the series G_{\sqcup} in Theorem 3.15. □

The shuffle brackets will be used to define shuffle regularized multiple Eisenstein series in the next chapter.

Chapter 4

Regularizations of multiple Eisenstein series

This chapter is devoted to Question 1 in the introduction, which was to find a regularization of the multiple Eisenstein series. We want to present two type of regularization: The shuffle regularized multiple Eisenstein series ([BT], [Ba2]) and stuffle regularized multiple Eisenstein series ([Ba2]).

The definition of shuffle regularized multiple Eisenstein series uses a beautiful connection of the Fourier expansion of multiple Eisenstein series and the coproduct of formal iterated integrals. The other regularization, the stuffle regularized multiple Eisenstein series uses the construction of the Fourier expansion of multiple Eisenstein series together with a result on regularization of multitangent functions by O. Bouillot ([Bo]).

We start by reviewing the definition of formal iterated integrals and the coproduct defined by Goncharov. An explicit example in length two will make the above mentioned connection of multiple Eisenstein series and this coproduct clear. After doing this, we give the definition of shuffle and stuffle regularized multiple Eisenstein series as presented in [BT] and [Ba2]. At the end of this chapter we compare these two regularizations with a help of a few examples.

4.1 Formal iterated integrals

Following Goncharov (Section 2 in [G]) we consider the algebra \mathcal{I} generated by the elements

$$\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1}), \quad a_i \in \{0, 1\}, N \geq 0.$$

together with the following relations

i) For any $a, b \in \{0, 1\}$ the unit is given by $\mathbb{I}(a; b) := \mathbb{I}(a; \emptyset; b) = 1$.

ii) The product is given by the shuffle product \sqcup

$$\begin{aligned} & \mathbb{I}(a_0; a_1, \dots, a_M; a_{M+N+1}) \mathbb{I}(a_0; a_{M+1}, \dots, a_{M+N}; a_{M+N+1}) \\ &= \sum_{\sigma \in sh_{M,N}} \mathbb{I}(a_0; a_{\sigma^{-1}(1)}, \dots, a_{\sigma^{-1}(M+N)}; a_{M+N+1}), \end{aligned}$$

where $sh_{M,N}$ is the set of $\sigma \in \mathfrak{S}_{M+N}$ such that $\sigma(1) < \dots < \sigma(M)$ and $\sigma(M+1) < \dots < \sigma(M+N)$.

iii) The path composition formula holds: for any $N \geq 0$ and $a_i, x \in \{0, 1\}$, one has

$$\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1}) = \sum_{k=0}^N \mathbb{I}(a_0; a_1, \dots, a_k; x) \mathbb{I}(x; a_{k+1}, \dots, a_N; a_{N+1}).$$

iv) For $N \geq 1$ and $a_i, a \in \{0, 1\}$ it is $\mathbb{I}(a; a_1, \dots, a_N; a) = 0$.

v) The path inversion is satisfied:

$$\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1}) = (-1)^N \mathbb{I}(a_{N+1}; a_N, \dots, a_1; a_0).$$

Definition 4.2. (Coproduct) Define the coproduct Δ on \mathcal{I} by

$$\begin{aligned} & \Delta(\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1})) := \\ & \sum \left(\mathbb{I}(a_0; a_{i_1}, \dots, a_{i_k}; a_{N+1}) \otimes \prod_{p=0}^k \mathbb{I}(a_{i_p}; a_{i_{p+1}}, \dots, a_{i_{p+1}-1}; a_{i_{p+1}}) \right), \end{aligned}$$

where the sum on the right runs over all $i_0 = 0 < i_1 < \dots < i_k < i_{k+1} = N+1$ with $0 \leq k \leq N$.

Proposition 4.1. ([G, Prop. 2.2]) The triple $(\mathcal{I}, \sqcup, \Delta)$ is a commutative graded Hopf algebra over \mathbb{Q} .

To calculate $\Delta(\mathbb{I}(a_0; a_1, \dots, a_8; a_9))$ one sums over all possible diagrams of the following form.

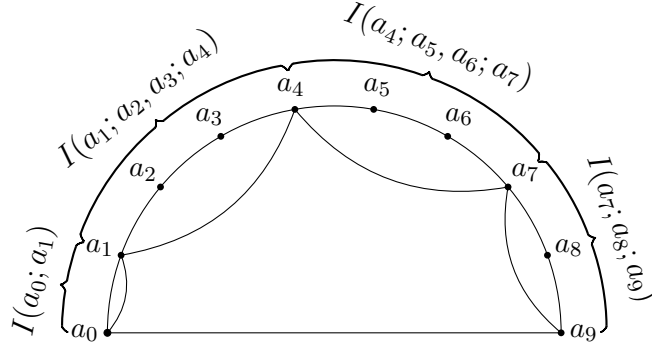


Figure 4.1: One diagram for the calculation of $\Delta(\mathbb{I}(a_0; a_1, \dots, a_8; a_9))$. It gives the term $I(a_0; a_1, a_4, a_7; a_9) \otimes I(a_0; a_1)I(a_1; a_2, a_3; a_4)I(a_4; a_5, a_6; a_7)I(a_7; a_8; a_9)$.

For our purpose it will be important to consider the quotient space¹

$$\mathcal{I}^1 = \mathcal{I}/\mathbb{I}(1; 0; 0)\mathcal{I}.$$

Let us denote by

$$I(a_0; a_1, \dots, a_N; a_{N+1})$$

an image of $\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1})$ in \mathcal{I}^1 . The quotient map $\mathcal{I} \rightarrow \mathcal{I}^1$ induces a Hopf algebra structure on \mathcal{I}^1 , but for our application we just need that for any $w_1, w_2 \in \mathcal{I}^1$, one has $\Delta(w_1 \sqcup w_2) = \Delta(w_1) \sqcup \Delta(w_2)$. The coproduct on \mathcal{I}^1 is given by the same formula as before by replacing \mathbb{I} with I . For integers $n \geq 0, s_1, \dots, s_r \geq 1$, we set

$$I_n(s_1, \dots, s_r) := I(1; \underbrace{0, 0, \dots, 1}_{s_1}, \dots, \underbrace{0, 0, \dots, 1}_{s_r}, \underbrace{0, \dots, 0}_n; 1).$$

In particular, we write $I(s_1, \dots, s_r)$ to denote² $I_0(s_1, \dots, s_r)$.

Proposition 4.2. ([BT, Eq. (3.5),(3.6) and Prop. 3.5])

i) We have $I_n(\emptyset) = 0$ if $n \geq 1$ or 1 if $n = 0$.

¹If one likes to interpret the integrals as real integrals, then the passage from \mathcal{I} to \mathcal{I}^1 regularizes these integrals such that $-\log(0) = \int_{1>t>0} \frac{dt}{t} := 0$.

²This notion fits well with the iterated integral expression of multiple zeta values. Recall that

$$\zeta(2, 3) = \int_{1>t_1>\dots>t_5>0} \underbrace{\frac{dt_1}{t_1} \cdot \frac{dt_2}{1-t_2}}_2 \cdot \underbrace{\frac{dt_3}{t_3} \cdot \frac{dt_4}{t_4} \cdot \frac{dt_5}{1-t_5}}_3.$$

This corresponds to $I(2, 3)$ (but is of course not the same since the I are formal symbols).

ii) For integers $n \geq 0, s_1, \dots, s_r \geq 1$,

$$I_n(s_1, \dots, s_r) = (-1)^n \sum^* \left(\prod_{j=1}^r \binom{k_j - 1}{s_j - 1} \right) I(k_1, \dots, k_r),$$

where the sum runs over all $k_1 + \dots + k_r = s_1 + \dots + s_r + n$ with $k_1, \dots, k_r \geq 1$.

iii) The set $\{I(s_1, \dots, s_r) \mid r \geq 0, s_i \geq 1\}$ forms a basis of the space \mathcal{I}^1 .

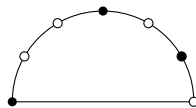
We give an example for ii): In \mathcal{I}^1 it is $I(1; 0; 0) = 0$ and therefore

$$\begin{aligned} 0 &= I(1; 0; 0)I(1; 0, 1; 0) \\ &= I(1; 0, 0, 1; 0) + I(1; 0, 0, 1; 0) + I(1; 0, 1, 0; 0) \\ &= 2I(3) + I_1(2) \end{aligned}$$

which gives $I_1(2) = -2I(3) = (-1)^1 \binom{2}{1} I(3)$.

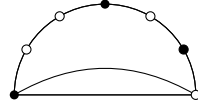
Remark 4.3. Statement iii) in Proposition 4.3 basically states that we can identify \mathcal{I}^1 with \mathfrak{H}^1 by sending $I(s_1, \dots, s_l)$ to $z_{s_1} \dots z_{s_l}$. In other words we can equip \mathfrak{H}^1 with the coproduct Δ . Instead of working with I we will use this identification in the next section, when defining the shuffle regularized multiple Eisenstein series.

Example 4.4. In the following we are going to calculate $\Delta(I(3, 2)) = \Delta(I(1; 0, 0, 1, 0, 1; 0))$. Therefore we have to determine all possible markings of the diagram



where the corresponding summand in the coproduct does not vanish. For simplicity we draw \circ to denote a 0 and \bullet to denote a 1. We will consider the $4 = 2^2$ ways of marking the two \bullet in the top part of the circle separately. As mentioned in the introduction, we want to compare the coproduct to the Fourier expansion of multiple Eisenstein series. Therefore, in this case we also calculate the expansion of $G_{3,2}(\tau)$ using the construction described in Section 1.2. Recall that we also had the 4 different parts $G_{3,2}^{RR}$, $G_{3,2}^{UR}$, $G_{3,2}^{RU}$ and $G_{3,2}^{UU}$. We will see that the number and positions of the marked \bullet correspond to the number and positions of the letter U in the word w of G^w .

i) Diagrams with no marked \bullet :

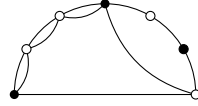


Corresponding sum in the coproduct:

$$I(0; \emptyset; 1) \otimes I(1; 0, 1, 0, 0, 1; 0) = 1 \otimes I(2, 3).$$

The part of the Fourier expansion of $G_{3,2}$ which is associated to this, is the one with no U "occurring", i.e. $G_{3,2}^{RR}(\tau) = \zeta(3, 2)$.

ii) Diagrams with the first \bullet marked:

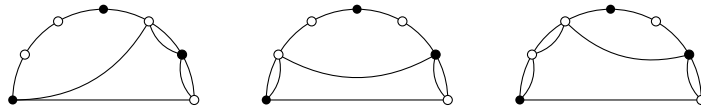


Corresponding sum in the coproduct:

$$I(1; 0, 0, 1; 0) \otimes \left(I(1; 0) \cdot I(0; 0) \cdot I(0; 1) \cdot I(1; 0, 1; 0) \right) = I(3) \otimes I(2).$$

The associated part of the Fourier expansion of $G_{3,2}$ is $G_{3,2}^{UR}(\tau) = g_3(\tau) \cdot \zeta(2)$.

iii) Diagrams with the second \bullet marked:



Corresponding sum in the coproduct:

$$\begin{aligned} & I(1; 0, 1; 0) \otimes \left(I(1; 0, 0, 1; 0) \cdot I(0; 1) \cdot I(1; 0) \right) \\ & + I(1; 0, 1; 0) \otimes \left(I(1; 0) \cdot I(0; 0, 1, 0; 1) \cdot I(1; 0) \right) \\ & + I(1; 0, 0, 1; 0) \otimes \left(I(1; 0) \cdot I(0; 0) \cdot I(0; 1, 0; 1) \cdot I(1; 0) \right) \\ & = I(2) \otimes I(3) - I(2) \otimes I_1(2) + I(3) \otimes I(2), \end{aligned}$$

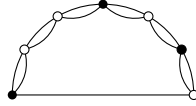
where we used $I(0, 0, 1, 0; 1) = -I_1(2)$ and $I(0; 1, 0; 1) = (-1)^2 I(1; 0, 1; 0) = I(2)$. Together with $I_1(2) = -2I(3)$ this gives

$$3I(2) \otimes I(3) + I(3) \otimes I(2).$$

Also the associated part of the Fourier expansion is the most complicated one. We had $G_{3,2}^{RU}(\tau) = \sum_{m>0} \Psi_{3,2}(m\tau)$ and with (1.6) we derived $\Psi_{3,2}(x) = 3\Psi_2(x) \cdot \zeta(3) + \Psi_3(x) \cdot \zeta(2)$, i.e.

$$G_{3,2}^{RU}(\tau) = 3g_2(\tau) \cdot \zeta(3) + g_3(\tau) \cdot \zeta(2).$$

iv) Diagrams with both \bullet marked:



Corresponding sum in the coproduct: $I(2, 3) \otimes 1$. The associated part of the Fourier expansion of $G_{3,2}$ is $G_{3,2}^{UU}(\tau) = g_{3,2}(\tau)$.

Summing all 4 parts together we obtain for the coproduct

$$\Delta(I(3, 2)) = 1 \otimes I(2, 3) + 3I(2) \otimes I(3) + 2I(3) \otimes I(2) + I(2, 3) \otimes 1$$

and for the Fourier expansion of $G_{2,3}(\tau)$:

$$G_{3,2}(\tau) = \zeta(3, 2) + 3g_2(\tau)\zeta(3) + 2g_3(\tau)\zeta(2) + g_{3,2}(\tau).$$

This shows that the left factors of the terms in the coproduct corresponds to the functions g and the right factors to the multiple zeta values. We will use this in the next section to define shuffle regularized multiple Eisenstein series.

4.3 Shuffle regularized multiple Eisenstein series

In this section we present the definition of shuffle regularized multiple Eisenstein series as it was done in [BT] together with the simplification developed in [Ba2]. We use the observation of the section before and use the coproduct Δ of formal iterated integrals to define these series. As mentioned in Remark 4.4 we can equip the space \mathfrak{H}^1 with

the coproduct Δ instead of working with the space \mathcal{I}^1 . Denote by $\mathcal{MZB} \subset \mathbb{C}[[q]]$ the space of all formal power series in q which can be written as a \mathbb{Q} -linear combination of products of multiple zeta values, powers of $(-2\pi i)$ and bi-brackets. In the following, we set $q = \exp(2\pi i\tau)$ with τ being an element in the upper half-plane. Since the coefficient of bi-brackets just have polynomial growth, the elements in \mathcal{MZB} and \mathcal{BD} can be viewed as holomorphic functions in the upper half-plane with this identification.

In analogy to the map $Z^\sqcup : (\mathfrak{H}^1, \sqcup) \rightarrow \mathcal{MZ}$ of shuffle regularized multiple zeta values (Proposition 1.2), the map $\mathfrak{g}^\sqcup : (\mathfrak{H}^1, \sqcup) \rightarrow \mathbb{Q}[2\pi i][[q]]$ defined on the generators $z_{t_1} \dots z_{t_l}$ by

$$\mathfrak{g}^\sqcup(z_{t_1} \dots z_{t_m}) = g_{t_1+\dots+t_m}^\sqcup(\tau) := (-2\pi i)^{t_1+\dots+t_m} [t_1, \dots, t_m]^\sqcup,$$

is also an algebra homomorphism by Theorem 3.15.

With this notation we can recall the definition of G^\sqcup from [Ba2] (which is a variant of the definition in [BT], where the authors did not use bi-brackets and the shuffle bracket).

Definition 4.4. For integers $s_1, \dots, s_l \geq 1$, define the functions $G_{s_1, \dots, s_l}^\sqcup(\tau) \in \mathcal{MZB}$, called *shuffle regularized multiple Eisenstein series*, as

$$G_{s_1, \dots, s_l}^\sqcup(\tau) := m \left((Z^\sqcup \otimes \mathfrak{g}^\sqcup) \circ \Delta(z_{s_1} \dots z_{s_l}) \right),$$

where m denotes the multiplication given by $m : a \otimes b \mapsto a \cdot b$.

We can view G^\sqcup as an algebra homomorphism $G^\sqcup : (\mathfrak{H}^1, \sqcup) \rightarrow \mathcal{MZB}$ such that the following diagram commutes

$$\begin{array}{ccc} (\mathfrak{H}^1, \sqcup) & \xrightarrow{\Delta} & (\mathfrak{H}^1, \sqcup) \otimes (\mathfrak{H}^1, \sqcup) \\ G^\sqcup \downarrow & & \downarrow Z^\sqcup \otimes \mathfrak{g}^\sqcup \\ \mathcal{MZB} & \xleftarrow{m} & \mathcal{MZ} \otimes \mathbb{Q}[2\pi i][[q]] \end{array}$$

Theorem 4.5. ([Ba2, Thm. 6.5], [BT, Thm. 1.1, 1.2]) For all $s_1, \dots, s_l \geq 1$ the shuffle regularized multiple Eisenstein series $G_{s_1, \dots, s_l}^\sqcup$ have the following properties:

- i) They are holomorphic functions on the upper half-plane having a Fourier expansion with the shuffle regularized multiple zeta values as the constant term.
- ii) They fulfill the shuffle product.
- iii) For integers $s_1, \dots, s_l \geq 2$ they equal the multiple Eisenstein series

$$G_{s_1, \dots, s_l}^\sqcup(\tau) = G_{s_1, \dots, s_l}(\tau)$$

and therefore they fulfill the shuffle product in these cases.

□

Parts i) and ii) in this theorem follow directly by definition. The important part here is iii), which states that the connection of the Fourier expansion and the coproduct, as illustrated in Example 4.5, holds in general. It also proves that the shuffle regularized multiple Eisenstein series fulfill the stuffle product in many cases. Though the exact failure of the stuffle product of these series is unknown so far.

4.5 Stuffle regularized multiple Eisenstein series

Motivated by the calculation of the Fourier expansion of multiple Eisenstein series described in Section 1.2 we consider the following construction.

Construction 4.6. Given a \mathbb{Q} -algebra (A, \cdot) and a family of homomorphism

$$\{w \mapsto f_w(m)\}_{m \in \mathbb{N}}$$

from $(\mathfrak{H}^1, *)$ to (A, \cdot) , we define for $w \in \mathfrak{H}^1$ and $M \in \mathbb{N}$

$$F_w(M) := \sum_{\substack{1 \leq k \leq l(w) \\ w_1 \dots w_k = w \\ M > m_1 > \dots > m_k > 0}} f_{w_1}(m_1) \dots f_{w_k}(m_k) \in A,$$

where $l(w)$ denotes the length of the word w and $w_1 \dots w_k = w$ is a decomposition of w into k words in \mathfrak{H}^1 .

Proposition 4.7. ([Ba2, Prop. 6.8]) For all $M \in \mathbb{N}$ the assignment $w \mapsto F_w(M)$, described above, determines an algebra homomorphism from $(\mathfrak{H}^1, *)$ to (A, \cdot) . In particular $\{w \mapsto F_w(m)\}_{m \in \mathbb{N}}$ is again a family of homomorphism as used in Construction 4.8. □

For a word $w = z_{s_1} \dots z_{s_l} \in \mathfrak{H}^1$ we also write in the following $f_{s_1, \dots, s_l}(m) := f_w(m)$ and similarly $F_{s_1, \dots, s_l}(M) := F_w(M)$.

Example 4.8. Let $f_w(m)$ be as in Construction 4.8. In small lengths the F_w are given by

$$F_{s_1}(M) = \sum_{M > m_1 > 0} f_{s_1}(m_1), \quad F_{s_1, s_2}(M) = \sum_{M > m_1 > 0} f_{s_1, s_2}(m_1) + \sum_{M > m_1 > m_2 > 0} f_{s_1}(m_1) f_{s_2}(m_2)$$

and one can check directly by the use of the stuffle product for the f_w that

$$\begin{aligned}
 F_{s_1}(M) \cdot F_{s_2}(M) &= \sum_{M > m_1 > 0} f_{s_1}(m_1) \cdot \sum_{M > m_2 > 0} f_{s_2}(m_2) \\
 &= \sum_{M > m_1 > m_2 > 0} f_{s_1}(m_1) f_{s_2}(m_2) + \sum_{M > m_2 > m_1 > 0} f_{s_2}(m_2) f_{s_1}(m_1) + \sum_{M > m_1 > 0} f_{s_1}(m_1) f_{s_2}(m_1) \\
 &= \sum_{M > m_1 > m_2 > 0} f_{s_1}(m_1) f_{s_2}(m_2) + \sum_{M > m_2 > m_1 > 0} f_{s_2}(m_2) f_{s_1}(m_1) \\
 &+ \sum_{M > m_1 > 0} (f_{s_1, s_2}(m_1) + f_{s_2, s_1}(m_1) + f_{s_1 + s_2}(m_1)) \\
 &= F_{s_1, s_2}(M) + F_{s_2, s_1}(M) + F_{s_1 + s_2}(M).
 \end{aligned}$$

Let us now give an explicit example for maps f_w in which we are interested. Recall (Definition 1.5) that for integers $s_1, \dots, s_l \geq 2$ we defined the multitangent function by

$$\Psi_{s_1, \dots, s_l}(z) = \sum_{\substack{n_1 > \dots > n_l \\ n_j \in \mathbb{Z}}} \frac{1}{(z + n_1)^{s_1} \cdots (z + n_l)^{s_l}}.$$

In [Bo], where these functions were introduced, the author uses the notation $\mathcal{T}e^{s_1, \dots, s_l}(z)$ which corresponds to our notation $\Psi_{s_1, \dots, s_l}(z)$. It was shown there that the series $\Psi_{s_1, \dots, s_l}(z)$ converges absolutely when $s_1, \dots, s_l \geq 2$. These functions fulfill (for the cases they are defined) the stuffle product. As explained in Section 1.2 the multitangent functions appear in the calculation of the Fourier expansion of the multiple Eisenstein series G_{s_1, \dots, s_l} , for example in length two it is

$$G_{s_1, s_2}(\tau) = \zeta(s_1, s_2) + \zeta(s_1) \sum_{m_1 > 0} \Psi_{s_2}(m_1 \tau) + \sum_{m_1 > 0} \Psi_{s_1, s_2}(m_1 \tau) + \sum_{m_1 > m_2 > 0} \Psi_{s_1}(m_1 \tau) \Psi_{s_2}(m_2 \tau).$$

One nice result of [Bo] is a regularization of the multitangent function to get a definition of $\Psi_{s_1, \dots, s_l}(z)$ for all $s_1, \dots, s_l \in \mathbb{N}$. We will use this result together with the above construction to recover the Fourier expansion of the multiple Eisenstein series.

Theorem 4.9. ([Bo]) For all $s_1, \dots, s_l \in \mathbb{N}$ there exist holomorphic functions Ψ_{s_1, \dots, s_l} on \mathbb{H} with the following properties

- i) Setting $q = e^{2\pi i \tau}$ for $\tau \in \mathbb{H}$ the map $w \mapsto \Psi_w(\tau)$ defines an algebra homomorphism from $(\mathfrak{H}^1, *)$ to $(\mathbb{C}[[q]], \cdot)$.
- ii) In the case $s_1, \dots, s_l \geq 2$ the Ψ_{s_1, \dots, s_l} are given by the multitangent functions in Definition 1.5.

iii) The monotangents functions have the q -expansion given by

$$\Psi_1(\tau) = \frac{\pi}{\tan(\pi\tau)} = (-2\pi i) \left(\frac{1}{2} + \sum_{n>0} q^n \right), \quad \Psi_k(\tau) = \frac{(-2\pi i)^k}{(k-1)!} \sum_{n>0} n^{k-1} q^n \text{ for } k \geq 2.$$

iv) (Reduction into monotangent function) Every $\Psi_{s_1, \dots, s_l}(\tau)$ can be written as a \mathcal{MZ} -linear combination of monotangent functions. There are explicit $\epsilon_{i,k}^{s_1, \dots, s_l} \in \mathcal{MZ}$ s.th.

$$\Psi_{s_1, \dots, s_l}(\tau) = \delta^{s_1, \dots, s_l} + \sum_{i=1}^l \sum_{k=1}^{s_i} \epsilon_{i,k}^{s_1, \dots, s_l} \Psi_k(\tau),$$

where $\delta^{s_1, \dots, s_l} = \frac{(\pi i)^l}{l!}$ if $s_1 = \dots = s_l = 1$ and l even and $\delta^{s_1, \dots, s_l} = 0$ otherwise. For $s_1 > 1$ and $s_l > 1$ the sum on the right starts at $k = 2$, i.e. there are no $\Psi_1(\tau)$ appearing and therefore there is no constant term in the q -expansion.

Proof. This is just a summary of the results in Section 6 and 7 of [Bo]. The last statement iv) is given by Theorem 6 in [Bo]. \square

Due to iv) in the Theorem the calculation of the Fourier expansion of multiple Eisenstein series, where ordered sums of multitangent functions appear, reduces to ordered sums of monotangent functions. The connection of these sums to the brackets, i.e. to the functions g , is given by the following fact which can be seen by using iii) of the above Theorem. For $n_1, \dots, n_r \geq 2$ it is

$$g_{s_1, \dots, s_r}(\tau) = \sum_{m_1 > \dots > m_l > 0} \Psi_{s_1}(m_1\tau) \dots \Psi_{s_l}(m_l\tau).$$

For $w \in \mathfrak{H}^1$ we now use the Construction 4.8 with $A = \mathbb{C}[[q]]$ and the family of homomorphism $\{w \mapsto \Psi_w(n\tau)\}_{n \in \mathbb{N}}$ (See Theorem 4.11 i)) to define

$$\mathfrak{g}^{*,M}(w) := (-2\pi i)^{|w|} \sum_{\substack{1 \leq k \leq l(w) \\ w_1 \dots w_k = w}} \sum_{M > m_1 > \dots > m_k > 0} \Psi_{w_1}(m_1\tau) \dots \Psi_{w_k}(m_k\tau).$$

From Proposition 4.9 it follows that for all $M \in \mathbb{N}$ the map $\mathfrak{g}^{*,M}$ is an algebra homomorphism from $(\mathfrak{H}^1, *)$ to $\mathbb{C}[[q]]$.

To define stuffle regularized multiple Eisenstein series we need the following: For an arbitrary quasi-shuffle algebra $\mathbb{Q}\langle A \rangle$ define the following coproduct for a word w

$$\Delta_H(w) = \sum_{uv=w} u \otimes v.$$

Then it is known due to Hoffman ([H]) that the space $(\mathbb{Q}\langle A \rangle, \odot, \Delta_H)$ has the structure of a bialgebra. With this we try to mimic the definition of the G^{\sqcup} and use the coproduct structure on the space $(\mathfrak{H}^1, *, \Delta_H)$ to define for $M \geq 0$ the function $G^{*,M}$ and then take the limit $M \rightarrow \infty$ to obtain the stuffle regularized multiple Eisenstein series. For this we consider the following diagram

$$\begin{array}{ccc} (\mathfrak{H}^1, *) & \xrightarrow{\Delta_H} & (\mathfrak{H}^1, *) \otimes (\mathfrak{H}^1, *) \\ G^{*,M} \downarrow & & \downarrow \mathfrak{g}^{*,M} \otimes Z^* \\ \mathbb{C}[[q]] & \xleftarrow{m} & \mathbb{C}[[q]] \otimes \mathcal{MZ} \end{array}$$

with the above algebra homomorphism $\mathfrak{g}^{*,M} : (\mathfrak{H}^1, *) \rightarrow \mathbb{C}[[q]]$.

Definition 4.6. For integers $s_1, \dots, s_l \geq 1$ and $M \geq 1$, we define the q -series $G_{s_1, \dots, s_l}^{*,M} \in \mathbb{C}[[q]]$ as the image of the word $w = z_{s_1} \dots z_{s_l} \in \mathfrak{H}^1$ under the algebra homomorphism $(Z^* \otimes \mathfrak{g}^{*,M}) \circ \Delta_H$:

$$G_{s_1, \dots, s_l}^{*,M}(\tau) := m \left((\mathfrak{g}^{*,M} \otimes Z^*) \circ \Delta_H(w) \right) \in \mathbb{C}[[q]].$$

For $s_1, \dots, s_l \geq 2$ the limit

$$G_{s_1, \dots, s_l}^*(\tau) := \lim_{M \rightarrow \infty} G_{s_1, \dots, s_l}^{*,M}(\tau) \quad (4.1)$$

exists and we have $G_{s_1, \dots, s_l} = G_{s_1, \dots, s_l}^* = G_{s_1, \dots, s_l}^{\sqcup}$ ([Ba2, Prop. 6.13]).

Remark 4.10. The open question is for what general s_1, \dots, s_l the limit in (4.1) exists. It is believed that this is exactly the case for $s_1 \geq 2$ and $s_2, \dots, s_l \geq 1$ as explained in Remark 6.14 in [Ba2]. This would be the case if $\Psi_{1, \dots, 1}$ are the only multitangent functions with a constant term in the decomposition of Theorem 4.11 iv). That this is the case is remarked, without a proof, in [Bo2] in the last sentence of page 3.

Theorem 11. ([Ba2]) For all $s_1, \dots, s_l \in \mathbb{N}$ and $M \in \mathbb{N}$ the $G_{s_1, \dots, s_l}^{*,M} \in \mathbb{C}[[q]]$ have the following properties:

- i) Their product can be expressed in terms of the stuffle product.
- ii) In the case where the limit $G_{s_1, \dots, s_l}^* := \lim_{M \rightarrow \infty} G_{s_1, \dots, s_l}^{*,M}$ exists, the functions G_{s_1, \dots, s_l}^* are elements in \mathcal{MZB} .
- iii) For $s_1, \dots, s_l \geq 2$ the G_{s_1, \dots, s_l}^* exist and equal the classical multiple Eisenstein series

$$G_{s_1, \dots, s_l}(\tau) = G_{s_1, \dots, s_l}^*(\tau).$$

4.7 Double shuffle relations for regularized multiple Eisenstein series

By Theorem 4.7 we know that the product of two shuffle regularized multiple Eisenstein series $G_{s_1, \dots, s_l}^{\sqcup}$ with $s_1, \dots, s_l \geq 1$ can be expressed by using the shuffle product formula. This means we can for example replace every ζ by G^{\sqcup} in the shuffle product (0.4) of multiple zeta values and obtain

$$G_2^{\sqcup} \cdot G_3^{\sqcup} = G_{2,3}^{\sqcup} + 3G_{3,2}^{\sqcup} + 6G_{4,1}^{\sqcup}. \quad (4.2)$$

Due to Theorem 4.7 iii) we know that $G_{s_1, \dots, s_l}^{\sqcup} = G_{s_1, \dots, s_l}$ whenever $s_1, \dots, s_l \geq 2$. Since the product of two multiple Eisenstein series G_{s_1, \dots, s_l} can be expressed using the stuffle product formula we also have

$$\begin{aligned} G_2^{\sqcup} \cdot G_3^{\sqcup} &= G_2 \cdot G_3 = G_{2,3} + G_{3,2} + G_5 \\ &= G_{2,3}^{\sqcup} + G_{3,2}^{\sqcup} + G_5^{\sqcup}. \end{aligned} \quad (4.3)$$

Combining (4.2) and (4.3) we obtain the relation $G_5^{\sqcup} = 2G_{3,2}^{\sqcup} + 6G_{4,1}^{\sqcup}$. In the following we will call these relations, i.e. the relations obtained by writing the product of two $G_{s_1, \dots, s_l}^{\sqcup}$ with $s_1, \dots, s_l \geq 2$ as the stuffle and shuffle product, *restricted double shuffle relations*.

We know that multiple zeta values fulfill even more linear relations, in particular we can express the product of two multiple zeta values $\zeta(s_1, \dots, s_l)$ in two different ways whenever $s_1 \geq 2$ and $s_2, \dots, s_l \geq 1$. A natural question therefore is, in which cases the G^{\sqcup} also fulfill these additional relations. The answer to this question is that some are satisfied and some are not, as the following will show.

In [Ba2, Example 6.15] it is shown that $G_{2,1,2}^{\sqcup} = G_{2,1,2}^*$, $G_{2,1}^{\sqcup} = G_{2,1}^*$, $G_{2,2,1}^{\sqcup} = G_{2,2,1}^*$ and $G_{4,1}^{\sqcup} = G_{4,1}^*$. Since the product of two G^* can be expressed using the stuffle product we obtain

$$\begin{aligned} G_2^{\sqcup} \cdot G_{2,1}^{\sqcup} &= G_2^* \cdot G_{2,1}^* \\ &= G_{2,1,2}^* + 2G_{2,2,1}^* + G_{4,1}^* + G_{2,3}^* \\ &= G_{2,1,2}^{\sqcup} + 2G_{2,2,1}^{\sqcup} + G_{4,1}^{\sqcup} + G_{2,3}^{\sqcup}. \end{aligned} \quad (4.4)$$

Using also the shuffle product to express $G_2^{\sqcup} \cdot G_{2,1}^{\sqcup}$ we obtain a linear relation in weight 5 which is not covered by the restricted double shuffle relations. This linear relation was numerically observed in [BT] but could not be proven there. So far it is not known exactly

which products of the G^{\sqcup} can be written in terms of stuffle products.

We end this chapter by comparing different versions of the double shuffle relations and explain, why multiple Eisenstein series can't fulfill every double shuffle relation of multiple zeta values. For this we write for words $u, v \in \mathfrak{H}^1$

$$\text{ds}(u, v) := u \sqcup v - u * v \in \mathfrak{H}^1.$$

Recall that by \mathfrak{H}^0 we denote the algebra of all admissible words, i.e. $\mathfrak{H}^0 = 1 \cdot \mathbb{Q} + x\mathfrak{H}y$. Additionally we set $\mathfrak{H}^2 = \mathbb{Q}\langle\{z_2, z_3, \dots\}\rangle$ to be the span of all words in \mathfrak{H}^1 with no z_1 occurring, i.e. the words for which the multiple Eisenstein series G exists. These are also the words for which the product of two multiple Eisenstein series can be expressed as the shuffle and stuffle product by Theorem 4.7. Denote by $|w| \in \mathfrak{H}^1$ the length of the word w with respect to the alphabet $\{x, y\}$ and define

$$\begin{aligned} \text{eds}_k &:= \left\{ \text{ds}(u, v) \in \mathfrak{H}^0 \mid |u| + |v| = k, u \in \mathfrak{H}^0, v \in \mathfrak{H}^0 \cup \{z_1\} \right\}, \\ \text{fds}_k &:= \left\{ \text{ds}(u, v) \in \mathfrak{H}^0 \mid |u| + |v| = k, u, v \in \mathfrak{H}^0 \right\}, \\ \text{rds}_k &:= \left\{ \text{ds}(u, v) \in \mathfrak{H}^0 \mid |u| + |v| = k, u, v \in \mathfrak{H}^2 \right\}. \end{aligned}$$

Also set $\text{eds} = \bigcup_{k>0} \text{eds}_k$ and similarly fds and rds . These spaces can be seen as the words in \mathfrak{H}^0 corresponding to the extended¹-, finite- and the restricted double shuffle relations. We have the inclusions

$$\text{rds}_k \subset \text{fds}_k \subset \text{eds}_k.$$

View ζ as a map $\mathfrak{H}^0 \rightarrow \mathcal{MZ}$ by sending the word $z_{s_1} \dots z_{s_l}$ to $\zeta(s_1, \dots, s_l)$. It is known ([IKZ, Thm. 2]), that eds_k is in the kernel of the map ζ and it is expected (Statement (3) after Conjecture 1 in [IKZ]) that actually $\text{eds}_k = \ker(\zeta)$. Viewing G^{\sqcup} in a similar way as a map $\mathfrak{H}^0 \rightarrow \mathcal{MZB}$, we know that rds_k is contained in the kernel of this map (Theorem 4.7 iv)). But due to (0.8) we also have $\text{ds}(z_2, z_2 z_1) \in \ker(G^{\sqcup})$ which is not an element of rds_5 . In [Ba] Example 6.15 ii) it is shown that there are also elements in $\text{fds}_k \subset \text{eds}_k$, that are not in the kernel of G^{\sqcup} . We therefore expect

$$\text{rds} \subsetneq \ker G^{\sqcup} \subsetneq \text{eds}$$

¹In [IKZ] the authors introduced the notion of extended double shuffle relations. We use this notion here for smaller subset of these relations given there as the relations described in statement (3) on page 315.

and the above examples show, that it seems to be crucial to understand for which indices we have $G^{\sqcup} = G^*$ to answer these questions.

We now discuss applications of the extended double shuffle relations to the classical theory of (quasi-)modular forms. As we have seen in the introduction it is known due to Euler that

$$\zeta(2)^2 = \frac{5}{2}\zeta(4), \quad \zeta(4)^2 = \frac{7}{6}\zeta(8), \quad \zeta(6)^2 = \frac{715}{691}\zeta(12). \quad (4.5)$$

In the following, we want to show how to prove these relations using extended double shuffle relations and argue why for multiple Eisenstein series the second is fulfilled but the first and the last equation of (4.5) are not.

- i) The relation $\zeta(2)^2 = \frac{5}{2}\zeta(4)$ can be proven in the following way by using double shuffle relations. It is $z_2 * z_2 = 2 \operatorname{ds}(z_3, z_1) - \frac{1}{2} \operatorname{ds}(z_2, z_2) + \frac{5}{2}z_4$, since

$$\begin{aligned} \operatorname{ds}(z_3, z_1) &= z_3z_1 + z_2z_2 - z_4, \\ \operatorname{ds}(z_2, z_2) &= 4z_3z_1 - z_4, \\ z_2 * z_2 &= 2z_2z_2 + z_4. \end{aligned}$$

Applying the map ζ we therefore deduce

$$\zeta(2)^2 = \zeta(z_2 * z_2) = \zeta\left(2 \operatorname{ds}(z_3, z_1) - \frac{1}{2} \operatorname{ds}(z_2, z_2) + \frac{5}{2}z_4\right) = \frac{5}{2}\zeta(4).$$

This relation is not true for Eisenstein series. Though $\operatorname{ds}(z_2, z_2)$ is in the kernel of G^{\sqcup} the element $\operatorname{ds}(z_3, z_1)$ is not. In fact, using the explicit formula for the Fourier expansion of $G_{3,1}^{\sqcup}$ and $G_{2,2}^{\sqcup}$ together with Proposition 2.12 for $d[2]$ we obtain $G^{\sqcup}(\operatorname{ds}(z_3, z_1)) = 6\zeta(2) dG_2$, where as before $d = q \frac{d}{dq}$. Using this we get

$$G_2^2 = G^{\sqcup}(z_2 * z_2) = G^{\sqcup}\left(2 \operatorname{ds}(z_3, z_1) - \frac{1}{2} \operatorname{ds}(z_2, z_2) + \frac{5}{2}z_4\right) = 12\zeta(2) dG_2 + \frac{5}{2}G_4.$$

This is a well-known fact in the theory of quasi-modular forms ([Za]).

- ii) Similarly to the above example one can prove the relation $\zeta(4)^2 = \frac{7}{6}\zeta(8)$ by checking that

$$z_4 * z_4 = \frac{2}{3} \operatorname{ds}(z_4, z_4) - \frac{1}{2} \operatorname{ds}(z_3, z_5) + \frac{7}{6}z_8$$

and since $\operatorname{ds}(z_4, z_4), \operatorname{ds}(z_3, z_5) \in \mathbf{rds}_8 \subset \ker G^{\sqcup}$ we also derive $G_4^2 = \frac{7}{6}G_8$ by applying the map G^{\sqcup} to this equation.

iii) To prove the relation $\zeta(6)^2 = \frac{715}{691}\zeta(12)$ in addition to the double shuffles of the form $\text{ds}(z_a, z_b)$ double shuffles of the form $\text{ds}(z_a z_b, z_c)$ are needed as well. This follows indirectly from the results obtained in [GKZ]. Using the computer one can check that

$$z_6 * z_6 = 2z_6 z_6 + z_{12} = \frac{715}{691} z_{12} + \frac{1}{2^2 \cdot 19 \cdot 113 \cdot 691} \cdot (R + E)$$

with $R \in \text{rds}_{12}$ and $E \in \text{eds}_{12} \setminus \text{rds}_{12}$ being the quite complicated elements

$$\begin{aligned} R = & 2005598 \text{ ds}(z_6, z_6) - 8733254 \text{ ds}(z_7, z_5) + 8128450 \text{ ds}(z_8, z_4) + 5121589 \text{ ds}(z_9, z_3) \\ & + 16364863 \text{ ds}(z_{10}, z_2) + 2657760 \text{ ds}(z_2 z_8, z_2) + 5220600 \text{ ds}(z_3 z_7, z_2) \\ & + 12711531 \text{ ds}(z_4 z_6, z_2) + 10460184 \text{ ds}(z_5 z_5, z_2) + 18601119 \text{ ds}(z_6 z_4, z_2) \\ & + 33877826 \text{ ds}(z_7 z_3, z_2) + 39496002 \text{ ds}(z_8 z_2, z_2) - 13288800 \text{ ds}(z_2 z_2, z_8) \\ & - 5220600 \text{ ds}(z_2 z_7, z_3) - 5734750 \text{ ds}(z_3 z_6, z_3) - 84659 \text{ ds}(z_4 z_5, z_3) \\ & + 2820467 \text{ ds}(z_5 z_4, z_3) - 5486485 \text{ ds}(z_6 z_3, z_3) + 8462489 \text{ ds}(z_7 z_2, z_3) \\ & - 6067131 \text{ ds}(z_2 z_6, z_4) - 7532671 \text{ ds}(z_3 z_5, z_4) - 10879336 \text{ ds}(z_4 z_3, z_5) \\ & - 5151234 \text{ ds}(z_4 z_4, z_4) + 3440519 \text{ ds}(z_5 z_3, z_4) - 1458819 \text{ ds}(z_6 z_2, z_4) \\ & + 2259096 \text{ ds}(z_5 z_2, z_5) - 4319105 \text{ ds}(z_3 z_4, z_5) - 778598 \text{ ds}(z_5 z_2, z_5) \\ & + 7609581 \text{ ds}(z_2 z_4, z_6) + 13064898 \text{ ds}(z_3 z_3, z_6) - 1281420 \text{ ds}(z_3 z_2, z_7), \end{aligned}$$

$$\begin{aligned} E = & -22681134 \text{ ds}(z_{11}, z_1) + 10631040 \text{ ds}(z_3 z_8, z_1) + 4241200 \text{ ds}(z_7 z_1, z_4) \\ & + 31893120 \text{ ds}(z_4 z_7, z_1) + 58185960 \text{ ds}(z_5 z_6, z_1) + 78309000 \text{ ds}(z_6 z_5, z_1) \\ & + 77976780 \text{ ds}(z_7 z_4, z_1) + 44849700 \text{ ds}(z_8 z_3, z_1) - 13288800 \text{ ds}(z_9 z_2, z_1) \\ & - 15946560 \text{ ds}(z_{10} z_1, z_1) + 75052824 \text{ ds}(z_9 z_1, z_2) + 19477164 \text{ ds}(z_8 z_1, z_3) \\ & - 12951740 \text{ ds}(z_6 z_1, z_5) - 10631040 \text{ ds}(z_2 z_1, z_9) \end{aligned}$$

Here the elements E and R are in the kernel of ζ but E , in contrast to R , is not in the kernel of G^ω . The defect here is given by the cusp form Δ in weight 12 as one can derive

$$G^\omega(E) = -\frac{2147}{1200}(-2\pi i)^{12} \Delta.$$

It is still an open problem how to derive these Euler relations in general by using double shuffle relations. The last example shows that this also seems to be very complicated. But as the examples above show, this might be of great interest to understand the connection of modular forms and multiple zeta values. This together with the question which double

shuffle relations are fulfilled by multiple Eisenstein series will be considered in upcoming works by the author.

Chapter 5

q -analogues of multiple zeta values

In general, a q -analogue of an mathematical object is a generalization involving a new parameter q that returns the original object in the limit as $q \rightarrow 1$. The easiest example of such an generalization is the q -analogue of a natural number $n \in \mathbb{N}$ given by

$$[n]_q := \frac{1 - q^n}{1 - q} = 1 + q + \cdots + q^{n-1}.$$

Clearly this gives back the original number n as $\lim_{q \rightarrow 1} [n]_q = n$.

Several different models for q -analogues of multiple zeta values have been studied in recent years. A good overview of them can be found in [Zh]. There are different motivations to study q -analogues of multiple zeta values.

That our brackets can be seen as q -analogue of multiple zeta values somehow occurred by accident since their original motivation was their appearance in the Fourier expansion of multiple Eisenstein series. But as turned out, seeing them as q -analogues gives a direct connection to multiple zeta values. In this chapter we first show how the brackets can be seen as a q -analogue of multiple zeta values and then discuss how one can obtain relations between multiple zeta values using the results obtained in [BK]. The second section will be devoted to connecting the brackets to other q -analogues.

5.1 Brackets as q -analogues of MZV and the map Z_k

Define for $k \in \mathbb{N}$ the map $Z_k : \mathbb{Q}[[q]] \rightarrow \mathbb{R} \cup \{\infty\}$ by

$$Z_k(f) = \lim_{q \rightarrow 1} (1 - q)^k f(q).$$

Since we have seen that the brackets can be written as

$$[s_1, \dots, s_l] = \frac{1}{(s_1 - 1)! \dots (s_l - 1)!} \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{q^{n_j} P_{s_j-1}(q^{n_j})}{(1 - q^{n_j})^{s_j}}$$

and using $P_{k-1}(1) = (k-1)!$ and interchanging the summation and the limit we derive ([BK, Prop. 6.4]), that for $s_1 > 1$, i.e. $[s_1, \dots, s_l] \in \mathfrak{qMZ}$

$$Z_k([s_1, \dots, s_l]) = \begin{cases} \zeta(s_1, \dots, s_l), & k = s_1 + \dots + s_l, \\ 0, & k > s_1 + \dots + s_l. \end{cases}$$

Due to $\mathcal{MD} = \mathfrak{qMZ}[[1]]$ (Theorem 2.11) we can define a well-defined map¹ on the whole space \mathcal{MD} by

$$\begin{aligned} Z_k^{alg} : \text{Fil}_k^{\mathbb{W}}(\mathcal{MD}) &\rightarrow \mathbb{R}[T] \\ Z_k^{alg} \left(\sum_{j=0}^k g_j [1]^{k-j} \right) &= \sum_{j=0}^k Z_j(g_j) T^{k-j} \in \mathbb{R}[T] \end{aligned}$$

where $g_j \in \text{Fil}_j^{\mathbb{W}}(\mathfrak{qMZ})$.

Every relation between multiple zeta values of weight k is contained in the kernel of the map Z_k . Therefore the kernel of Z_k was studied in [BK].

Theorem 5.1. ([BK, Thm. 1.13]) For the kernel of $Z_k^{alg} \in \text{Fil}_k^{\mathbb{W}}(\mathcal{MD})$ we have

- i) If for $[s_1, \dots, s_l]$ it holds $s_1 + \dots + s_l < k$, then $Z_k^{alg}[s_1, \dots, s_l] = 0$.
- ii) For any $f \in \text{Fil}_{k-2}^{\mathbb{W}}(\mathcal{MD})$ we have $Z_k^{alg} d(f) = 0$, i.e., $d \text{Fil}_{k-2}^{\mathbb{W}}(\mathcal{MD}) \subseteq \ker Z_k$.
- iii) If $f \in \text{Fil}_k^{\mathbb{W}}(\mathcal{MD})$ is a cusp form for $\text{SL}_2(\mathbb{Z})$, then $Z_k^{alg}(f) = 0$.

Example 5.2. We illustrate some applications for Theorem 5.1. For this we recall identities for the derivatives and relations of brackets as they were given in [BK]. All of them can be obtained by using the results explained in Chapter 2.

$$d[1] = [3] + \frac{1}{2}[2] - [2, 1], \tag{5.1}$$

$$d[2] = [4] + 2[3] - \frac{1}{6}[2] - 4[3, 1], \tag{5.2}$$

$$d[2] = 2[4] + [3] + \frac{1}{6}[2] - 2[2, 2] - 2[3, 1], \tag{5.3}$$

$$d[1, 1] = [3, 1] + \frac{3}{2}[2, 1] + \frac{1}{2}[1, 2] + [1, 3] - 2[2, 1, 1] - [1, 2, 1], \tag{5.4}$$

$$[8] = \frac{1}{40}[4] - \frac{1}{252}[2] + 12[4, 4]. \tag{5.5}$$

¹This map is similar to the evaluation map $Z^* : \mathfrak{H}^1 \rightarrow \mathbb{R}[T]$, of stuffle regularized multiple zeta values, given in Proposition 1 in [IKZ]. We used this map in the previous chapters (Proposition 1.2) with $T = 0$.

Using Theorem 5.1 as immediate consequences and without any difficulties we recover the following well-known identities for multiple zeta values.

- i) If we apply Z_3 to (5.1) we deduce $\zeta(3) = \zeta(2, 1)$.
- ii) If we apply Z_4 to (5.2) and (5.3) we deduce $\zeta(4) = 4\zeta(3, 1) = \frac{4}{3}\zeta(2, 2)$.
- iii) The identity (5.4) reads in $q\mathcal{MZ}[1]$ as

$$d[1, 1] = \left([3] - [2, 1] + \frac{1}{2}[2] \right) \cdot [1] + 2[3, 1] - \frac{1}{2}[4] - \frac{1}{2}[2, 1] - \frac{1}{2}[3] + \frac{1}{3}[2].$$

Applying Z_4^{alg} we deduce again the two relations $\zeta(3) = \zeta(2, 1)$ and $4\zeta(3, 1) = \zeta(4)$, since by Theorem 5.1 we have

$$Z_4^{alg}(d[1, 1]) = (\zeta(3) - \zeta(2, 1))T - \frac{1}{2}\zeta(4) + 2\zeta(3, 1) = 0.$$

- iv) If we apply Z_8 to (5.5) we deduce $\zeta(8) = 12\zeta(4, 4)$.
- v) As we have seen in Proposition 2.13 the cusp form Δ can be written as

$$\begin{aligned} -\frac{1}{2^6 \cdot 5 \cdot 691}\Delta &= 168[5, 7] + 150[7, 5] + 28[9, 3] \\ &+ \frac{1}{1408}[2] - \frac{83}{14400}[4] + \frac{187}{6048}[6] - \frac{7}{120}[8] - \frac{5197}{691}[12]. \end{aligned} \quad (5.6)$$

Letting Z_{12} act on both sides of (5.6) one obtains the relation (0.6)

$$\frac{5197}{691}\zeta(12) = 168\zeta(5, 7) + 150\zeta(7, 5) + 28\zeta(9, 3).$$

But as mentioned in the introduction there are also elements in the kernel of Z_k that are not covered by Theorem 5.1. In weight 4 one has the relation of multiple zeta values $\zeta(4) = \zeta(2, 1, 1)$, i.e. it is $[4] - [2, 1, 1] \in \ker Z_4$. But this element can't be written as a linear combination of cusp forms, lower weight brackets or derivatives. But using the double shuffle relations for bi-brackets described in Section 3.2 one can prove¹ that

$$[4] - [2, 1, 1] = \frac{1}{2}(d[1] + d[2]) - \frac{1}{3}[2] - [3] + \begin{bmatrix} 2, 1 \\ 1, 0 \end{bmatrix}. \quad (5.7)$$

¹That the last term $\begin{bmatrix} 2, 1 \\ 1, 0 \end{bmatrix}$ in (5.7) is in the kernel of Z_4 can be proven in the following way: In Proposition 7.2 [BK] it is shown, that an element $f = \sum_{n>0} a_n q^n$ with $a_n = O(n^m)$ and $m < k - 1$ is in the kernel of Z_k . Here we have

$$\begin{bmatrix} 2, 1 \\ 1, 0 \end{bmatrix} = \sum_{\substack{u_1 > u_2 > 0 \\ v_1, v_2 > 0}} v_1 u_1 q^{v_1 u_1 + v_2 u_2} < \sum_{\substack{u_1, u_1 0 \\ v_1, v_2 > 0}} v_1 u_1 q^{v_1 u_1 + v_2 u_2} = d[1] \cdot [1],$$

where the $<$ is meant to be coefficient wise. Since the coefficients of $d[1] \cdot [1]$ grow like $n^2 \log(n)^2$ we conclude $\begin{bmatrix} 2, 1 \\ 1, 0 \end{bmatrix} \in \ker Z_4$.

Another way to see that many of the bi-brackets of weight k are in the kernel of the map Z_k is the following. Assume that $s_1 > r_1 + 1$ and $s_j \geq r_j + 1$ for $j = 2, \dots, l$, then using again the representation with the Eulerian polynomials (See also Proposition 1 [Zu]) we get

$$Z_{s_1+\dots+s_l} \left(\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \right) = \frac{1}{r_1! \dots r_l!} \zeta(s_1 - r_1, \dots, s_l - r_l)$$

and in particular with this assumption it is $\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \in \ker Z_{s_1+\dots+s_l+1}$.

The study of the kernel Z_k is of great interest since it contains every relation of weight k . We expect that every element in the kernel of Z_k can be described using bi-brackets of a "certain kind" and it seems to be a really interesting question to specify this "certain kind" explicitly. To determine which bi-brackets are exactly in the kernel of the map Z_k and also which bi-brackets can be written in terms of brackets in $q\mathcal{MZ}$ is an open problem. The naive guess, that exactly the bi-brackets $\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix}$ where at least one $r_j > 0$ are elements in the kernel of $Z_{s_1+\dots+s_l+r_1+\dots+r_l}$ is wrong, since for example

$$\lim_{q \rightarrow 1} (1 - q)^3 \begin{bmatrix} 1, 1 \\ 1, 0 \end{bmatrix} = \infty.$$

5.2 Connection to other q -analogues

In [Zh] the author gives an overview over several different q -analogues of multiple zeta values. Here we complement his work and focus on aspects related to our brackets. To compare the brackets to other q -analogues we first generalize the notion of a q -analogue of multiple zeta values as it was done in [BK2]. This notion of a q -analogue does cover many but not all q -analogues described in [Zh].

In the following we fix a subset $S \subset \mathbb{N}$, which we consider as the support for index entries, i.e. we assume $s_1, \dots, s_l \in S$. For each $s \in S$ we let $Q_s(t) \in \mathbb{Q}[t]$ be a polynomial with $Q_s(0) = 0$ and $Q_s(1) \neq 0$. We set $Q = \{Q_s(t)\}_{s \in S}$. A sum of the form

$$Z_Q(s_1, \dots, s_l) := \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{Q_{s_j}(q^{n_j})}{(1 - q^{n_j})^{s_j}} \quad (5.8)$$

with polynomials Q_s as before, defines a q -analogue of a multiple zeta-value of weight $k = s_1 + \dots + s_l$ and length l . Observe only because of $Q_{s_1}(0) = 0$ this defines an element of $\mathbb{Q}[[q]]$. That these objects are in fact a q -analogue of a multiple zeta-value is justified

by the following calculation.

$$\begin{aligned} \lim_{q \rightarrow 1} (1-q)^k Z_Q(s_1, \dots, s_l) &= \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \lim_{q \rightarrow 1} \left(Q_{s_j}(q^{n_j}) \frac{(1-q)^{s_j}}{(1-q^{n_j})^{s_j}} \right) \\ &= Q_{s_1}(1) \dots Q_{s_l}(1) \cdot \zeta(s_1, \dots, s_l). \end{aligned}$$

Here we used that $\lim_{q \rightarrow 1} (1-q)^s / (1-q^n)^s = 1/n^s$ and with the same arguments as in [BK] Proposition 6.4, the above interchange of the limit with the sum can be justified for all (s_1, \dots, s_l) with $s_1 > 1$. Related definitions for q -analogues of multiple zeta values are given in [Br], [Ta], [Zu2] and [OOZ]. It is convenient to define $Z_Q(\emptyset) = 1$ and then we denote the vector space spanned by all these elements by

$$Z(Q, S) := \left\langle Z_Q(s_1, \dots, s_l) \mid l \geq 0 \text{ and } s_1, \dots, s_l \in S \right\rangle_{\mathbb{Q}}. \quad (5.9)$$

Note by the above convention we have, that \mathbb{Q} is contained in this space.

Lemma 5.3. ([BK2, Lemma 2.1]) If for each $r, s \in S$ there exists numbers $\lambda_j(r, s) \in \mathbb{Q}$ such that

$$Q_r(t) \cdot Q_s(t) = \sum_{\substack{j \in S \\ 1 \leq j \leq r+s}} \lambda_j(r, s) (1-t)^{r+s-j} Q_j(t), \quad (5.10)$$

then the vector space $Z(Q, S)$ is a \mathbb{Q} -algebra. □

Theorem 5.4. ([BK2, Thm. 2.4]) Let $Z(Q, \mathbb{N}_{>1})$ be any family of q -analogues of multiple zeta values as in (5.9), where each $Q_s(t) \in \mathbb{Q}$ is a polynomial with degree at most $s-1$, then

$$Z(Q, \mathbb{N}_{>1}) = \mathcal{MD}^\sharp,$$

where \mathcal{MD}^\sharp was the in Section 2.2 defined subalgebra of \mathcal{MD} spanned by all brackets $[s_1, \dots, s_l]$ with $s_j \geq 2$. Therefore, all such families of q -analogues of multiple zeta values are \mathbb{Q} -subalgebras of \mathcal{MD} . □

The following proposition allows one to write an arbitrary element in $Z(Q, \mathbb{N}_{>1})$ as an linear combination of $[s_1, \dots, s_l] \in \mathcal{MD}^\sharp$.

Proposition 5.5. ([BK2, Prop. 2.5]) Assume $k \geq 2$. For $1 \leq i, j \leq k-1$ define the numbers $b_{i,j}^k \in \mathbb{Q}$ by

$$\sum_{j=1}^{k-1} \frac{b_{i,j}^k}{j!} t^j := \binom{t+k-1-i}{k-1}.$$

With this it is for $1 \leq i \leq k-1$ and $Q_j^E(t) = \frac{1}{(j-1)!} t P_j(t)$

$$t^i = \sum_{j=2}^k b_{i,j-1}^k (1-t)^{k-j} Q_j^E(t).$$

□

We give some examples of q -analogues of multiple zeta values, with some being of the above type.

i) To write the brackets in the above way we choose $Q_s^E(t) = \frac{1}{(s-1)!} t P_{s-1}(t)$, where the $P_s(t)$ are the Eulerian polynomials defined earlier by

$$\frac{t P_{s-1}(t)}{(1-t)^s} = \sum_{d=1}^{\infty} d^{s-1} t^d$$

for $s \geq 0$. With this we have for all $s_1, \dots, s_l \in \mathbb{N}$

$$[s_1, \dots, s_l] := \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{Q_{s_j}^E(q^{n_j})}{(1-q^{n_j})^{s_j}}.$$

and $\mathcal{MD} = Z(\{Q_s^E(t)\}_s, \mathbb{N})$.

ii) The polynomials $Q_s^T(t) = t^{s-1}$ are considered in [Ta],[Zu2] and sums of the form (5.8) with $s_1 > 1$ and $s_2, \dots, s_l \geq 1$ are studied there. Using Proposition 5.5 every q -analogue of this type can be written explicitly in terms of brackets.

iii) Okounkov chooses the following polynomials in [O]

$$Q_s^O(t) = \begin{cases} t^{\frac{s}{2}} & s = 2, 4, 6, \dots \\ t^{\frac{s-1}{2}}(1+t) & s = 3, 5, 7, \dots \end{cases}$$

and defines for $s_1, \dots, s_l \in S = \mathbb{N}_{>1}$

$$Z(s) = \sum_{n_1 > \dots > n_l > 0} \prod_{j=0}^l \frac{Q_{s_j}^O(q^{n_j})}{(1-q^{n_j})^{s_j}}.$$

We write for the space of the Okounkov q -multiple zetas

$$\mathfrak{qMZV} = Z(\{Q_s^O(t)\}_s, \mathbb{N}_{>1}).$$

Due to Theorem 5.4 we have $\mathfrak{qMZV} = \mathcal{MD}^\sharp$. In [O] Okounkov conjectures, that the space \mathfrak{qMZV} is closed under the operator d . In length 1 this is proven in Proposition 2.9 [BK2].

iv) There are also q -analogues which are not of the type as in (5.8). For example, the model introduced in [OOZ] and further studied in [MMEF]. For $s_1, \dots, s_l \geq 1$ they are define by

$$\mathfrak{z}_q(s_1, \dots, s_l) = \sum_{n_1 > \dots > n_l > 0} \frac{q^{n_1}}{(1 - q^{n_1})^{s_1} \dots (1 - q^{n_l})^{s_l}}.$$

It is easy to see, that every $\mathfrak{z}_q(s_1, \dots, s_l)$ can be written in terms of bi-brackets. For example

$$\begin{aligned} \mathfrak{z}_q(2, 1) &= \sum_{n_1 > n_2 > 0} \frac{q^{n_1}}{(1 - q^{n_1})^2 (1 - q^{n_2})} = \sum_{n_1 > n_2 > 0} \frac{q^{n_1} (q^{n_2} + 1 - q^{n_2})}{(1 - q^{n_1})^2 (1 - q^{n_2})} \\ &= \sum_{n_1 > n_2 > 0} \frac{q^{n_1} q^{n_2}}{(1 - q^{n_1})^2 (1 - q^{n_2})} + \sum_{n_1 > n_2 > 0} \frac{q^{n_1}}{(1 - q^{n_1})^2} \\ &= [2, 1] + \sum_{n_1 > 0} \frac{(n_1 - 1) q^{n_1}}{(1 - q^{n_1})^2} = [2, 1] + \begin{bmatrix} 2 \\ 1 \end{bmatrix} - [2]. \end{aligned}$$

Similarly one can prove $\mathfrak{z}_q(2, 1, 1) = [2, 1, 1] - 2[2, 1] + \begin{bmatrix} 2, 1 \\ 1, 0 \end{bmatrix} + \begin{bmatrix} 2 \\ 2 \end{bmatrix} - \frac{3}{2} \begin{bmatrix} 2 \\ 1 \end{bmatrix} + [2]$. For higher weights this also works as illustrated in the following

$$\begin{aligned} \mathfrak{z}_q(2, 2) &= \sum_{n_1 > n_2 > 0} \frac{q^{n_1}}{(1 - q^{n_1})^2 (1 - q^{n_2})^2} = \sum_{n_1 > n_2 > 0} \frac{q^{n_1} (q^{n_2} + 1 - q^{n_2})}{(1 - q^{n_1})^2 (1 - q^{n_2})^2} \\ &= [2, 2] + \mathfrak{z}_q(2, 1) = [2, 2] + [2, 1] + \begin{bmatrix} 2 \\ 1 \end{bmatrix} - [2]. \end{aligned}$$

Using again Proposition 5.5 it becomes clear for arbitrary weights $s_1, \dots, s_l \geq 2$ we can write $\mathfrak{z}_q(s_1, \dots, s_l)$ in terms of bi-brackets.

Writing any q -analogue in terms of bi-brackets enables us to use the double shuffle structure explained in Chapter 3 to obtain linear relations for all of these q -analogues. This is still work in progress and is not part of this thesis.

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Bibliography

Appendices

Appendix A

The algebra of generating functions
for multiple divisor sums and
applications to multiple zeta values

The algebra of generating functions for multiple divisor sums and applications to multiple zeta values

HENRIK BACHMANN, ULF KÜHN

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Abstract

We study the algebra \mathcal{MD} of generating function for multiple divisor sums and its connections to multiple zeta values. The generating functions for multiple divisor sums are formal power series in q with coefficients in \mathbb{Q} arising from the calculation of the Fourier expansion of multiple Eisenstein series. We show that the algebra \mathcal{MD} is a filtered algebra equipped with a derivation and use this derivation to prove linear relations in \mathcal{MD} . The (quasi-)modular forms for the full modular group $SL_2(\mathbb{Z})$ constitute a subalgebra of \mathcal{MD} this also yields linear relations in \mathcal{MD} . Generating functions of multiple divisor sums can be seen as a q -analogue of multiple zeta values. Studying a certain map from this algebra into the real numbers we will derive a new explanation for relations between multiple zeta values, including those in length 2, coming from modular forms.

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1 Introduction

Multiple zeta values are natural generalizations of the Riemann zeta values that are defined for integers $s_1 > 1$ and $s_i \geq 1$ for $i > 1$ by

$$\zeta(s_1, \dots, s_l) := \sum_{n_1 > n_2 > \dots > n_l > 0} \frac{1}{n_1^{s_1} \dots n_l^{s_l}}.$$

Because of its occurrence in various fields of mathematics and physics these real numbers are of particular interest. The \mathbb{Q} -vector space of all multiple zeta values of weight k is then given by

$$\mathcal{MZ}_k := \langle \zeta(s_1, \dots, s_l) \mid s_1 + \dots + s_l = k \text{ and } l > 0 \rangle_{\mathbb{Q}}.$$

It is well known that the product of two multiple zeta values can be written as a linear combination of multiple zeta values of the same weight by using the stuffle or shuffle relations. Thus they generate a \mathbb{Q} -algebra \mathcal{MZ} . There are beautiful conjectures about the dimensions of finite dimensional subspaces of \mathcal{MZ} determined by the weight and the depth filtration.

In [GKZ] Gangl, Kaneko and Zagier introduced double Eisenstein series, which were generalized to multiple Eisenstein series in [Ba1]. These series are sums over certain positive sectors in the multiple product of a lattice. They give natural generalizations of the well-known Eisenstein series from the theory of modular forms similar as the multiple zeta values generalize special values of the Riemann zeta function. These functions do by construction satisfy the stuffle relations. But due to convergence problems the shuffle relation needs some modification; it seems to hold up to an error term which involves derivatives. The motivation behind this article is the idea to understand these corrections algebraically, although this will not be discussed here furthermore (c.f. [BBK], [BT]). It has been shown in [Ba1] that multiple Eisenstein series have a Fourier expansion, which decomposes as a \mathcal{MZ} -linear combination of generating functions for multiple divisor sums $[s_1, \dots, s_l]$ which we also refer to as brackets in this paper. For example the double Eisenstein series $G_{4,4}$ and the triple Eisenstein series $G_{3,2,2}$ are given by

$$\begin{aligned} G_{4,4}(\tau) &= \zeta(4, 4) + 20\zeta(6)(-2\pi i)^2[2](q_\tau) + 3\zeta(4)(-2\pi i)^4[4](q_\tau) + (-2\pi i)^8[4, 4](q_\tau), \\ G_{3,2,2}(\tau) &= \zeta(3, 2, 2) + \left(\frac{54}{5}\zeta(2, 3) + \frac{51}{5}\zeta(3, 2) \right) (-2\pi i)^2[2](q_\tau) + \frac{16}{3}\zeta(2, 2)(-2\pi i)^3[3](q_\tau) \\ &\quad + 3\zeta(3)(-2\pi i)^4[2, 2](q_\tau) + 4\zeta(2)(-2\pi i)^5[3, 2](q_\tau) + (-2\pi i)^7[3, 2, 2](q_\tau), \end{aligned}$$

where $\tau \in \mathbb{H}$, $q_\tau = \exp(2\pi i\tau)$ and the brackets $[s_1, \dots, s_l]$ are kind of a combinatorial object¹ that will be described now. As a generalization of the classical divisor

¹In [GKZ] certain linear combinations of these functions were called combinatorial Eisenstein series

sums we define for natural numbers $r_1, \dots, r_l \in \mathbb{N}_0 = \{0, 1, 2, \dots\}$ the *multiple divisor sum* by

$$\sigma_{r_1, \dots, r_l}(n) = \sum_{\substack{u_1 v_1 + \dots + u_l v_l = n \\ u_1 > \dots > u_l > 0}} v_1^{r_1} \dots v_l^{r_l}. \quad (1.1)$$

For any integers $s_1, \dots, s_l > 0$ the generating function for the multiple divisor sum $\sigma_{s_1-1, \dots, s_l-1}$ is defined by the formal power series

$$[s_1, \dots, s_l] := \frac{1}{(s_1 - 1)! \dots (s_l - 1)!} \sum_{n > 0} \sigma_{s_1-1, \dots, s_l-1}(n) q^n \in \mathbb{Q}[[q]].$$

Here and in the following, we will simply write $[s_1, \dots, s_l]$ instead of $[s_1, \dots, s_l](q)$. We refer to these generating functions of multiple divisor sums also as *brackets*.²

Example 1.1. We give a few examples:

$$\begin{aligned} [2] &= q + 3q^2 + 4q^3 + 7q^4 + 6q^5 + 12q^6 + 8q^7 + 15q^8 + \dots, \\ [4, 2] &= \frac{1}{6} (q^3 + 3q^4 + 15q^5 + 27q^6 + 78q^7 + 135q^8 + \dots), \\ [4, 4, 4] &= \frac{1}{216} (q^6 + 9q^7 + 45q^8 + 190q^9 + 642q^{10} + 1899q^{11} + \dots), \\ [3, 1, 3, 1] &= \frac{1}{4} (q^{10} + 2q^{11} + 8q^{12} + 16q^{13} + 43q^{14} + 70q^{15} + \dots), \\ [1, 2, 3, 4, 5] &= \frac{1}{288} (q^{15} + 17q^{16} + 107q^{17} + 512q^{18} + 1985q^{19} + \dots). \end{aligned}$$

Notice that the first non vanishing coefficient of q^n in $[s_1, \dots, s_l]$ appears at $n = \frac{l(l+1)}{2}$, because it belongs to the "smallest" possible partition

$$l \cdot 1 + (l-1) \cdot 1 + \dots + 1 \cdot 1 = n,$$

i.e. $u_j = j$ and $v_j = 1$ for $1 \leq j \leq l$. The number $k = s_1 + \dots + s_l$ is called the *weight* of $[s_1, \dots, s_l]$ and l denotes the *length*. These numbers satisfy $l \leq k$.

Definition 1.2. We define the vector space \mathcal{MD} to be the \mathbb{Q} vector space generated by $[\emptyset] = 1 \in \mathbb{Q}[[q]]$ and all brackets $[s_1, \dots, s_l]$. On \mathcal{MD} we have the increasing filtration $\text{Fil}_\bullet^{\text{W}}$ given by the weight and the increasing filtration $\text{Fil}_\bullet^{\text{L}}$ given by the length, i.e., we have

$$\begin{aligned} \text{Fil}_k^{\text{W}}(\mathcal{MD}) &:= \langle [s_1, \dots, s_l] \mid s_1 + \dots + s_l \leq k \rangle_{\mathbb{Q}} \\ \text{Fil}_l^{\text{L}}(\mathcal{MD}) &:= \langle [s_1, \dots, s_r] \mid r \leq l \rangle_{\mathbb{Q}}. \end{aligned}$$

² The brackets $[2, \dots, 2]$ were in the context of partitions already studied by P.A. MacMahon (see [Ma]) and named generalized divisor sums. It was shown in [AR] that these are quasi-modular forms, see also Remark 2.1

If we consider the length and weight filtration at the same time we use the short notation $\text{Fil}_{k,l}^{\text{W,L}} := \text{Fil}_k^{\text{W}} \text{Fil}_l^{\text{L}}$. As usual we set

$$\begin{aligned} \text{gr}_k^{\text{W}}(\mathcal{MD}) &:= \text{Fil}_k^{\text{W}}(\mathcal{MD}) / \text{Fil}_{k-1}^{\text{W}}(\mathcal{MD}) \\ \text{gr}_l^{\text{L}}(\mathcal{MD}) &:= \text{Fil}_l^{\text{L}}(\mathcal{MD}) / \text{Fil}_{l-1}^{\text{L}}(\mathcal{MD}). \end{aligned}$$

and as above $\text{gr}_{k,l}^{\text{W,L}} := \text{gr}_k^{\text{W}} \text{gr}_l^{\text{L}}$.

For example for even $k \geq 4$ the Eisenstein series G_k , which are well-known to be modular forms of weight k for the group $\text{SL}_2(\mathbb{Z})$, are elements in this vector spaces, because they satisfy

$$G_k = \frac{\zeta(k)}{(-2\pi i)^k} + \frac{1}{(k-1)!} \sum_{n>0} \sigma_{k-1}(n) q^n = -\frac{1}{2} \frac{B_k}{k!} [\emptyset] + [k] \in \text{Fil}_k^{\text{W}}(\mathcal{MD}),$$

also the quasi-modular form G_2 of weight 2 is an element of $\text{Fil}_2^{\text{W}}(\mathcal{MD})$. Our first result is

Theorem 1.3. *The \mathbb{Q} -vector space \mathcal{MD} has the structure of a bifiltered \mathbb{Q} -Algebra $(\mathcal{MD}, \cdot, \text{Fil}_{\bullet}^{\text{W}}, \text{Fil}_{\bullet}^{\text{L}})$, where the multiplication is the natural multiplication of formal power series and the filtrations $\text{Fil}_{\bullet}^{\text{W}}$ and $\text{Fil}_{\bullet}^{\text{L}}$ are induced by the weight and length, in particular*

$$\text{Fil}_{k_1,l_1}^{\text{W,L}}(\mathcal{MD}) \cdot \text{Fil}_{k_2,l_2}^{\text{W,L}}(\mathcal{MD}) \subset \text{Fil}_{k_1+k_2,l_1+l_2}^{\text{W,L}}(\mathcal{MD}).$$

Remark 1.4. In fact we prove that this product on \mathcal{MD} is a quasi-shuffle product in the sense of Hofmann and Ihara [HI].

Example 1.5. The first products of brackets are given by

$$[1] \cdot [1] = 2[1, 1] + [2] - [1], \quad (1.2)$$

$$[1] \cdot [2] = [1, 2] + [2, 1] + [3] - \frac{1}{2}[2], \quad (1.3)$$

$$[1] \cdot [2, 1] = [1, 2, 1] + 2[2, 1, 1] - \frac{3}{2}[2, 1] + [2, 2] + [3, 1]. \quad (1.4)$$

For small weight k or at least a small l length we can compute a sufficiently large number of the Fourier coefficients of a bracket. We can therefore determine lower bounds for the number of linearly independent elements in $\text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD})$, in order to do so we need to check that the matrix of with rows given by the Fourier coefficients of each element has a sufficient high rank.

Theorem 1.6. We have the following exact values or lower bounds for $\dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD})$

Appendix A. The algebra of generating functions for multiple divisor sums and applications to multiple zeta values

$k \setminus l$	0	1	2	3	4	5	6	7	8	9	10	11
0	1											
1	1	2										
2	1	3	4									
4	1	4	7	8								
3	1	5	10	14	15							
5	1	6	14	22	27	28						
6	1	7	18	32	44	50	51					
7	1	8	23	44	67	84	91	92				
8	1	9	28	59	97	133	156	164	165			
9	1	10	34	76	135	200	254	284	293	294		
10	1	11	40	97	183	290	396	474	512	522	523	
11	1	12	47	120	242	408	594	760	869	916	927	928
12	1	13	54	147	313	559	?	?	?	?	?	?
13	1	14	62	177	398	?	?	?	?	?	?	?
14	1	15	70	212	498	?	?	?	?	?	?	?
15	1	16	79	249	?	?	?	?	?	?	?	?

Table 1: $\dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD})$: **exact value**, **lower bound**

The number of generators of $\text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD})$ is easily calculated, thus giving an upper bound for the dimension of this space is equivalent to give a lower bound for the number of relations in the generators of $\text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD})$. The equalities come from the fact that we know enough relations in the cases marked black in Table 1.

For the multiple zeta values conjecturally all linear relations are due the fact that the shuffle and the stuffle relations give two different description of the product of two multiple zeta values, albeit in practice there are different methods to prove distinct relations like the cyclic sum identity [HO] or the Zagier-Ohno relation [OZ]. So far we know only one way to write a product of two brackets as a linear combination in \mathcal{MD} and this doesn't suffice to give linear relations between elements in \mathcal{MD} . However, as we will see now, \mathcal{MD} has the additional structure of a differential algebra and moreover there are several ways to express the derivative of a bracket. By now linear relations in \mathcal{MD} are proved either by using derivatives and or the theory of quasi-modular forms.

Theorem 1.7. The operator $d = q \frac{d}{dq}$ is a derivation on \mathcal{MD} , it maps $\text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD})$ to $\text{Fil}_{k+2,l+1}^{\text{W,L}}(\mathcal{MD})$.

Our proof actually allows us to derive explicit formulas for $d[s_1]$ and $d[s_1, s_2]$.

Remark 1.8. Our formula for $d[k]$ may be seen as the Euler decomposition formula for \mathcal{MD} , since for we prove in Proposition 3.3 that for $s_1 + s_2 = k + 2$

$$[s_1] \cdot [s_2] = \sum_{a+b=k+2} \left(\binom{a-1}{s_1-1} + \binom{a-1}{s_2-1} \right) [a, b] - \binom{k}{s_1-1} [k+1] + \binom{k}{s_1-1} \frac{d[k]}{k}.$$

Frankly speaking the derivative $d[k]$ measures the failure of the shuffle relation for the product of two length one bracket.

We will show now how to derive from these formulas non trivial linear relations.

Example 1.9. (Relations from derivatives) The first derivatives are given by

$$d[1] = [3] + \frac{1}{2}[2] - [2, 1], \quad (1.5)$$

$$d[2] = [4] + 2[3] - \frac{1}{6}[2] - 4[3, 1], \quad (1.6)$$

$$d[2] = 2[4] + [3] + \frac{1}{6}[2] - 2[2, 2] - 2[3, 1], \quad (1.7)$$

$$d[1, 1] = [3, 1] + \frac{3}{2}[2, 1] + \frac{1}{2}[1, 2] + [1, 3] - 2[2, 1, 1] - [1, 2, 1]. \quad (1.8)$$

The difference of (1.6) and (1.7) leads to the first linear relation in $\text{Fil}_4^{\text{W}}(\mathcal{MD})$:

$$[4] = 2[2, 2] - 2[3, 1] + [3] - \frac{1}{3}[2]. \quad (1.9)$$

Example 1.10. (Leibniz rule) Since d is a derivation it satisfies the Leibniz rule, e.g., because of (1.2)

$$d[1] \cdot [1] + [1] \cdot d[1] = d([1] \cdot [1]) = d(2[1, 1] + [2] - [1]).$$

Now using (1.5), (1.6) and (1.8) together with the explicit description of the various products we could alternatively prove the relation (1.9).

Example 1.11. (Relations from modular forms) It is a well-known fact from the theory of modular forms that $G_4^2 = \frac{7}{6}G_8$ because the space of weight 8 modular forms for $\text{SL}_2(\mathbb{Z})$ is one dimensional. We therefore have

$$\frac{1}{720}[4] + [4] \cdot [4] = \frac{7}{6}[8].$$

Using the product as described in Proposition 2.8 we get

$$[4] \cdot [4] = 2[4, 4] + [8] + \frac{1}{360}[4] - \frac{1}{1512}[2],$$

which then gives the following relation in $\text{Fil}_8^{\text{W}}(\mathcal{MD})$:

$$[8] = \frac{1}{40}[4] - \frac{1}{252}[2] + 12[4, 4]. \quad (1.10)$$

Beside the methods mentioned in Example 1.9 and 1.11 other obvious ways to get relations in weight k are either to multiply a relation in weight l by a bracket of weight $k - l$ or to take the derivative of a relation in weight $k - 2$.

Example 1.12. (Relations from known relations) If we multiply the relation (1.9) in weight 4 with [2], then we obtain in $\text{Fil}_6^{\text{W}}(\mathcal{MD})$:

$$\begin{aligned} [6] = & \frac{1}{20}[2] - \frac{1}{12}[3] - \frac{1}{4}[4] + [5] - \frac{4}{3}[2, 2] + \frac{1}{6}[3, 1] + [2, 3] + 2[3, 2] \\ & + 6[2, 2, 2] - 2[3, 1, 2] - 2[2, 3, 1] - 2[3, 2, 1] + [2, 4] - 2[3, 3] + [4, 2] - 2[5, 1]. \end{aligned} \quad (1.11)$$

If we apply d to the relation (1.9) in weight 4, then we obtain in $\text{Fil}_6^{\text{W}}(\mathcal{MD})$:

$$\begin{aligned} [6] = & \frac{1}{20}[2] - \frac{3}{4}[3] + \frac{11}{4}[4] - 3[5] - \frac{2}{3}[2, 2] + \frac{3}{2}[3, 1] + 4[2, 3] + 2[2, 4] \\ & + 5[3, 2] - 18[4, 1] + 5[4, 2] + 6[5, 1] - 8[2, 3, 1] - 8[3, 1, 2] - 2[3, 2, 1] + 18[4, 1, 1]. \end{aligned} \quad (1.12)$$

In order to study the linear relations in the generators of \mathcal{MD} systematically it is better first to understand some of the algebra structure of \mathcal{MD} . For this purpose we call a brackets $[s_1, \dots, s_l]$ admissible, if $s_1 > 1$. We show that the vector space qMZ of admissible brackets is a sub algebra of \mathcal{MD} . In addition we prove that \mathcal{MD} is a polynomial ring over qMZ with indeterminate [1], i.e. we have

$$\mathcal{MD} = \text{qMZ}[[1]]$$

(see Theorem 2.14). With this structure in our hands it is easy see that it suffices to study the linear relations in the generators of the quotient spaces $\text{gr}_{k,l}^{\text{W,L}}(\text{qMZ})$ in order to get upper bounds on the dimensions of all the graded or filtrated pieces of qMZ or \mathcal{MD} . In Theorem 5.5 we present our results in this direction. We like to emphasize that the focus of this article is not to give the best possible results on the number of relations. We expect that with a more detailed study of the kind of relations we can obtain so far we could derive much better results and we plan to come back to this in future [Ba2].

The notation qMZ shall emphasize the relation to q-analogues of multiple zeta values, which will be explained now. Our algebra qMZ is related, but not isomorphic, to a recent modification of multiple q zeta values as proposed in [OT] or [Ta], see also Remark 6.1.

Define for $k \geq 0$ the map Z_k on $\text{Fil}_k^{\text{W}}(\text{qMZ})$ by

$$Z_k[s_1, \dots, s_l] = \lim_{q \rightarrow 1} (1 - q)^k [s_1, \dots, s_l].$$

We will show that with this definition we have

$$Z_k([s_1, \dots, s_l]) = \begin{cases} \zeta(s_1, \dots, s_l), & k = s_1 + \dots + s_l, \\ 0, & k > s_1 + \dots + s_l. \end{cases}$$

Since $\mathcal{MD} = \text{qMZ}[[1]]$ we can define a map $Z_k^{alg} : \text{Fil}_k^W(\mathcal{MD}) \rightarrow \mathbb{R}[T]$ by

$$Z_k^{alg} \left(\sum_{j=0}^k g_j [1]^{k-j} \right) = \sum_{j=0}^k Z_j(g_j) T^{k-j} \in \mathbb{R}[T]$$

where $g_j \in \text{Fil}_j^W(\text{qMZ})$. For our next result an analytical interpretation of Z_k^{alg} in a broader context is the key fact.

Theorem 1.13. For the kernel of $Z_k^{alg} \in \text{Fil}_k^W(\mathcal{MD})$ we have

- i) If for $[s_1, \dots, s_l]$ it holds $s_1 + \dots + s_l < k$, then $Z_k^{alg}[s_1, \dots, s_l] = 0$.
- ii) For any $f \in \text{Fil}_{k-2}^W(\mathcal{MD})$ we have $Z_k^{alg} d(f) = 0$, i.e., $d \text{Fil}_{k-2}^W(\mathcal{MD}) \subseteq \ker Z_k$.
- iii) If $f \in \text{Fil}_k^W(\mathcal{MD})$ is a cusp form for $\text{SL}_2(\mathbb{Z})$, then $Z_k^{alg}(f) = 0$, i.e. $S_k(\text{SL}_2(\mathbb{Z})) \subseteq \ker Z_k$.

Using Theorem 1.13 we get as immediate consequences and without any difficulties the following well-known identities for multiple zeta values.

Example 1.14. i) If we apply Z_3 to (1.5) we deduce $\zeta(3) = \zeta(2, 1)$.

ii) If we apply Z_4 to (1.6) and (1.7) we deduce $\zeta(4) = 4\zeta(3, 1) = \frac{4}{3}\zeta(2, 2)$.

iii) The identity (1.8) reads in $\text{qMZ}[[1]]$ as

$$d[1, 1] = \left([3] - [2, 1] + \frac{1}{2}[2] \right) \cdot [1] + 2[3, 1] - \frac{1}{2}[4] - \frac{1}{2}[2, 1] - \frac{1}{2}[3] + \frac{1}{3}[2].$$

Applying Z_4^{alg} we deduce again the two relations $\zeta(3) = \zeta(2, 1)$ and $4\zeta(3, 1) = \zeta(4)$, since by Theorem 1.13 we have

$$Z_4^{alg}(d[1, 1]) = (\zeta(3) - \zeta(2, 1))T - \frac{1}{2}\zeta(4) + 2\zeta(3, 1) = 0.$$

iv) If we apply Z_8 to (1.10) we deduce $\zeta(8) = 12\zeta(4, 4)$.

v) As an application of Theorem 1.6 we can prove for the cusp form $\Delta \in S_{12}(\text{SL}_2(\mathbb{Z}))$ the representation

$$\begin{aligned} -\frac{1}{2^6 \cdot 5 \cdot 691} \Delta &= 168[5, 7] + 150[7, 5] + 28[9, 3] \\ &+ \frac{1}{1408}[2] - \frac{83}{14400}[4] + \frac{187}{6048}[6] - \frac{7}{120}[8] - \frac{5197}{691}[12]. \end{aligned} \quad (1.13)$$

Letting Z_{12} act on both sides of (1.13) one obtains the relation

$$\frac{5197}{691} \zeta(12) = 168\zeta(5, 7) + 150\zeta(7, 5) + 28\zeta(9, 3).$$

Finally we point to the fact that the last identity coming from the cusp form Δ has been obtained via period polynomials in [GKZ]. A remarkable fact of this relation is that it is not provable within the double shuffle relations in weight 12 and depth 2 alone, since also the extended double shuffle relations are needed for its proof. This article contains results that will be part of the dissertation project by the first author.

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2 The algebra of generating function of multiple divisor sums

The proof of Theorem 1.3 will occupy this section. First we consider products of polylogarithms at negative integers. This will give us an explicit formula for the product of two brackets.

Remark 2.1. We start with a remark on where brackets also have appeared before. In the following we will write $\{a\}^l$ for a length l sequence a, \dots, a .

- i) The sum in (1.1) can be interpreted as a sum over all partitions of n into l distinct parts \underline{u}_j . The v_j count the appearance of the parts \underline{u}_j . For example let $l = 2$, $n = 5$ and $r_1 = r_2 = 1$ then we have five partitions of 5 into 2 distinct parts:

$$\begin{aligned} 5 &= \underline{4} + \underline{1} = \underline{3} + \underline{2} = \underline{3} + \underline{1} + \underline{1} = \underline{2} + \underline{2} + \underline{1} = \underline{2} + \underline{1} + \underline{1} + \underline{1} \\ &= \underline{4} \cdot 1 + \underline{1} \cdot 1 = \underline{3} \cdot 1 + \underline{2} \cdot 1 = \underline{3} \cdot 1 + \underline{1} \cdot 2 = \underline{2} \cdot 2 + \underline{1} \cdot 1 = \underline{2} \cdot 1 + \underline{1} \cdot 3 \end{aligned}$$

and therefore $\sigma_{0,0}(5) = 5$ and $\sigma_{2,1}(5) = 1^2 \cdot 1^1 + 1^2 \cdot 1^1 + 1^2 \cdot 2^1 + 2^2 \cdot 1^1 + 1^2 \cdot 3^1 = 11$.

- ii) The multiple divisor sum $\sigma_{\{0\}^l}$ counts the number of partitions of n into l distinct parts. Therefore the generating function of the partition functions $p(n)$ which counts all partitions of n can be written as

$$\sum_{n>0} p(n)q^n = \sum_{l>0} [\{1\}^l].$$

- iii) The brackets $[2, \dots, 2]$ were already studied by P. A. MacMahon (see [Ma]) under the name of generalized divisor sums in the context of partitions. They were also studied in [AR] where it was also shown, that they are quasi-modular forms.

Definition 2.2. Recall that for $s, z \in \mathbb{C}$, $|z| < 1$ the polylogarithm $\text{Li}_s(z)$ of weight s is given by

$$\text{Li}_s(z) = \sum_{n>0} \frac{z^n}{n^s}.$$

We then define a *normalized polylogarithm* by

$$\tilde{\text{Li}}_{1-s}(z) := \frac{\text{Li}_{1-s}(z)}{\Gamma(s)}.$$

The normalized polylogarithm $\text{Li}_{1-s}(z)$ extends to an entire function in s and to a holomorphic function in z where $|z| < 1$. However for our purposes it is enough to know that for natural $s > 0$ this is a rational function in z with a pole at $z = 1$ (c.f. Remark 2.4). Now we can define brackets as functions in q .

Proposition 2.3. For $q \in \mathbb{C}$ with $|q| < 1$ and for all $s_1, \dots, s_l \in \mathbb{N}$ we can write the brackets as

$$[s_1, \dots, s_l] = \sum_{n_1 > \dots > n_l > 0} \tilde{\text{Li}}_{1-s_1}(q^{n_1}) \dots \tilde{\text{Li}}_{1-s_l}(q^{n_l}).$$

Proof. This follows directly from the definitions, see also Lemma 2.5. □

Remark 2.4. As mentioned above the polylogarithms $\text{Li}_{-s}(z)$ for $s \in \mathbb{N}$ are rational functions in z with a pole in $z = 1$. More precisely for $|z| < 1$ they can be written as

$$\text{Li}_{-s}(z) = \sum_{n>0} n^s z^n = \frac{z P_s(z)}{(1-z)^{s+1}}$$

where $P_s(z)$ is the s -th Eulerian polynomial. Such a polynomial is given by

$$P_s(X) = \sum_{n=0}^{s-1} A_{s,n} X^n,$$

where the Eulerian numbers $A_{s,n}$ are defined by

$$A_{s,n} = \sum_{i=0}^n (-1)^i \binom{s+1}{i} (n+1-i)^s.$$

Therefore the coefficients (the Eulerian numbers) of P_s are positive. It fulfills the relation

$$P_{k+1}(t) = P_k(t)(1+kt) + t(1-t)P'_k(t)$$

and therefore $P_k(1) = k!$. For proofs of all these properties see for example [Fo]. In particular the recursive formula can be found in [Fo] as equation (3.3). Proposition 2.6 then gives an expression for the product of Eulerian polynomials as rational linear combinations of polynomials in the form $(1-z)^j P_i(z)$ with $j, i \in \mathbb{N}$.

Lemma 2.5. For $s_1, \dots, s_l \in \mathbb{N}$ we have

$$[s_1, \dots, s_l] = \frac{1}{(s_1 - 1)! \dots (s_l - 1)!} \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{q^{n_j} P_{s_j-1}(q^{n_j})}{(1 - q^{n_j})^{s_j}},$$

where $P_k(t)$ is the k -th Eulerian polynomial.

Proof. The claim follows directly from Remark 2.4 because

$$\sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{q^{n_j} P_{s_j-1}(q^{n_j})}{(1 - q^{n_j})^{s_j}} = \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \sum_{v_j > 0} v_j^{s_j-1} q^{v_j n_j} = \sum_{n > 0} \sigma_{s_1-1, \dots, s_l-1}(n) q^n.$$

□

The product of $[s_1]$ and $[s_2]$ can thus be written as

$$\begin{aligned} [s_1] \cdot [s_2] &= \sum_{n_1 > n_2 > 0} \tilde{\text{Li}}_{1-s_1}(q^{n_1}) \tilde{\text{Li}}_{1-s_2}(q^{n_2}) + \sum_{n_2 > n_1 > 0} \dots + \sum_{n_1 = n_2 > 0} \tilde{\text{Li}}_{1-s_1}(q^{n_1}) \tilde{\text{Li}}_{1-s_2}(q^{n_1}) \\ &= [s_1, s_2] + [s_2, s_1] + \sum_{n > 0} \tilde{\text{Li}}_{1-s_1}(q^n) \tilde{\text{Li}}_{1-s_2}(q^n). \end{aligned}$$

In order to prove that this product is an element of $\text{Fil}_{s_1+s_2}^{\text{W}}(\mathcal{MD})$ the product $\tilde{\text{Li}}_{1-s_1}(q^n) \tilde{\text{Li}}_{1-s_2}(q^n)$ must be a rational linear combination of $\tilde{\text{Li}}_{1-j}(q^n)$ with $1 \leq j \leq s_1 + s_2$. We therefore need the following

Lemma 2.6. For $a, b \in \mathbb{N}$ we have

$$\tilde{\text{Li}}_{1-a}(z) \cdot \tilde{\text{Li}}_{1-b}(z) = \sum_{j=1}^a \lambda_{a,b}^j \tilde{\text{Li}}_{1-j}(z) + \sum_{j=1}^b \lambda_{b,a}^j \tilde{\text{Li}}_{1-j}(z) + \tilde{\text{Li}}_{1-(a+b)}(z),$$

where the coefficient $\lambda_{a,b}^j \in \mathbb{Q}$ for $1 \leq j \leq a$ is given by

$$\lambda_{a,b}^j = (-1)^{b-1} \binom{a+b-j-1}{a-j} \frac{B_{a+b-j}}{(a+b-j)!}.$$

Proof. We prove this by using the generating function

$$L(X) := \sum_{k > 0} \tilde{\text{Li}}_{1-k}(z) X^{k-1} = \sum_{k > 0} \sum_{n > 0} \frac{n^{k-1} z^n}{(k-1)!} X^{k-1} = \sum_{n > 0} e^{nX} z^n = \frac{e^X z}{1 - e^X z}.$$

With this one can see by direct calculation that

$$L(X) \cdot L(Y) = \frac{1}{e^{X-Y} - 1} L(X) + \frac{1}{e^{Y-X} - 1} L(Y).$$

By the definition of the Bernoulli numbers

$$\frac{X}{e^X - 1} = \sum_{n \geq 0} \frac{B_n}{n!} X^n$$

this can be written as

$$L(X) \cdot L(Y) = \sum_{n > 0} \frac{B_n}{n!} (X - Y)^{n-1} L(X) + \sum_{n > 0} \frac{B_n}{n!} (Y - X)^{n-1} L(Y) + \frac{L(X) - L(Y)}{X - Y}.$$

The statement then follows by calculating the coefficient of $X^{a-1}Y^{b-1}$ in this equation. \square

Example 2.7. We have $\lambda_{1,1}^1 = B_1 = -\frac{1}{2}$ and thus

$$\tilde{\text{Li}}_{1-1}(z) \cdot \tilde{\text{Li}}_{1-1}(z) = -\tilde{\text{Li}}_{1-1}(z) + \tilde{\text{Li}}_{1-2}(z).$$

Therefore the product $[1] \cdot [1]$ is given by

$$[1] \cdot [1] = 2[1, 1] + [2] - [1].$$

More generally, Lemma 2.6 implies the following explicit formula for the product in the length one case.

Proposition 2.8. We have the formula

$$[s_1] \cdot [s_2] = [s_1, s_2] + [s_2, s_1] + [s_1 + s_2] + \sum_{j=1}^{s_1} \lambda_{s_1, s_2}^j [j] + \sum_{j=1}^{s_2} \lambda_{s_2, s_1}^j [j].$$

Proof. This is a straightforward calculation \square

In order to prove Theorem 1.3 we need to show that the above considerations work in general and not only in the length 1 case. For this we use the notion of quasi-shuffle algebras ([HI]). Let $A = \{z_1, z_2, \dots\}$ be the set of letters z_j for each natural number $j \in \mathbb{N}$, $\mathbb{Q}A$ the \mathbb{Q} -vector space generated by these letters and $\mathbb{Q}\langle A \rangle$ the noncommutative polynomial algebra over \mathbb{Q} generated by words with letters in A . For a commutative and associative product \diamond on $\mathbb{Q}A$, $a, b \in A$ and $w, v \in \mathbb{Q}\langle A \rangle$ we define on $\mathbb{Q}\langle A \rangle$ recursively a product by $1 * w = w * 1 = w$ and

$$aw * bv := a(w * bv) + b(aw * v) + (a \diamond b)(w * v).$$

Equipped with this product one has the

Proposition 2.9. The vector space $\mathbb{Q}\langle A \rangle$ with the product $*$ is a commutative \mathbb{Q} -algebra.

Proof. See [HI] Theorem 2.1. □

Motivated by the product expression of the polylogarithms in Lemma 2.6 we define the product \diamond on $\mathbb{Q}A$ by

$$z_a \diamond z_b = \sum_{j=1}^a \lambda_{a,b}^j z_j + \sum_{j=1}^b \lambda_{b,a}^j z_j + z_{a+b}.$$

This is a commutative and associative product on $\mathbb{Q}A$, because it arises from the product of the pairwise linearly independent polylogarithms $\tilde{Li}_{1-t}(z)$ in Proposition 2.6, and therefore $(\mathbb{Q}\langle A \rangle, *)$ is a commutative \mathbb{Q} -algebra by Proposition 2.9 above. Theorem 1.3 now follows from the next proposition.

Proposition 2.10. For the linear map $[\cdot] : (\mathbb{Q}\langle A \rangle, *) \longrightarrow (\mathcal{MD}, \cdot)$ defined on the generators $w = z_{s_1} \dots z_{s_l}$ by $[w] := [s_1, \dots, s_l]$ we have

$$[w * v] = [w] \cdot [v]$$

and therefore \mathcal{MD} is a \mathbb{Q} -algebra and $[\cdot]$ an algebra homomorphism.

Proof. This follows by the same argument as in the multiple zeta value case, see e.g. [H1] Thm 3.2, by using induction on the length of the words w and v together with Proposition 2.6. □

Now we have proven Theorem 1.3. As a special case of this theorem we have the following explicit formula.

Example 2.11. For $a, b, c \in \mathbb{N}$ we have

$$\begin{aligned} [a] \cdot [b, c] &= [z_a * z_b z_c] = [z_a z_b z_c + z_b z_a z_c + z_b z_c z_a + z_b(z_a \diamond z_c) + (z_a \diamond z_b)z_c] \\ &= [a, b, c] + [b, a, c] + [b, c, a] + [a + b, c] + [b, a + c] \\ &\quad + \sum_{j=1}^a \lambda_{a,c}^j [b, j] + \sum_{j=1}^c \lambda_{c,a}^j [b, j] + \sum_{j=1}^a \lambda_{a,b}^j [j, c] + \sum_{j=1}^b \lambda_{b,a}^j [j, c]. \end{aligned}$$

We would like to point out another structure of the algebra \mathcal{MD} , which will be important later on when we consider the connection to multiple zeta values, and which was already mentioned in the introduction.

Definition 2.12. We define the set of all admissible brackets $\mathfrak{q}\mathcal{MZ}$ as the span of all brackets $[s_1, \dots, s_l]$ with $s_1 > 1$. With $\text{Fil}_{k,l}^{\mathfrak{W},\mathfrak{L}}(\mathfrak{q}\mathcal{MZ})$ we denote the admissible brackets of length l and weight k similar to the non-admissible case.

With this we have the

Theorem 2.13. The vector space $\mathfrak{q}\mathcal{MZ}$ is a subalgebra of \mathcal{MD} .

Proof. It is enough to show that \mathfrak{qMZ} is closed under multiplication. Let $f = [a, \dots]$ and $g = [b, \dots]$ be elements in \mathfrak{qMZ} , i.e. $a > 1$ and $b > 1$. Due to Proposition 2.10 we have

$$f \cdot g = [z_a w] \cdot [z_b v] = [z_a w * z_b v],$$

where $w, v \in \mathbb{Q}\langle A \rangle$ are words in the alphabet $A = \{z_1, z_2, \dots\}$. So in order to prove the statement we have to show that $z_a w * z_b v$ is a linear combination of words $z_c u \in \mathbb{Q}\langle A \rangle$ with $c > 1$ and arbitrary words $u \in \mathbb{Q}\langle A \rangle$. By the definition of the quasi-shuffle product $*$ we have

$$z_a w * z_b v = z_a(w * z_b v) + z_b(z_a w * v) + (z_a \diamond z_b)(w * v).$$

The first two summands clearly fulfill this condition, because we assumed $a, b > 1$, so it remains to show that $z_a \diamond z_b \in \mathbb{Q}A$ is a linear combination of letters z_j with $j > 1$. Again by definition we obtain

$$\begin{aligned} z_a \diamond z_b &= z_{a+b} + \sum_{j=1}^a \lambda_{a,b}^j z_j + \sum_{j=1}^b \lambda_{b,a}^j z_j \\ &= z_{a+b} + (\lambda_{a,b}^1 + \lambda_{b,a}^1) z_1 + \sum_{j=2}^a \lambda_{a,b}^j z_j + \sum_{j=2}^b \lambda_{b,a}^j z_j, \end{aligned}$$

so it suffices to show that $\lambda_{a,b}^1 + \lambda_{b,a}^1$ vanishes for $a, b > 1$. From the definition of $\lambda_{a,b}^j$ in Lemma 2.6 it is easy to see that

$$\lambda_{a,b}^1 + \lambda_{b,a}^1 = ((-1)^{a-1} + (-1)^{b-1}) \binom{a+b-2}{a-1} \frac{B_{a+b-1}}{(a+b-1)!}.$$

This term clearly vanishes when a and b have different parity. In the other case $a+b-1$ is odd and greater than 1, as $a, b > 1$. It is well known that in this case $B_{a+b-1} = 0$, from which we deduce that $\lambda_{a,b}^1 + \lambda_{b,a}^1 = 0$. \square

Theorem 2.14. i) We have $\mathcal{MD} = \mathfrak{qMZ}[1]$.

ii) The algebra \mathcal{MD} is a polynomial ring over \mathfrak{qMZ} with indeterminate $[1]$, i.e. \mathcal{MD} is isomorphic to $\mathfrak{qMZ}[T]$ by sending $[1]$ to T .

Proof. i) First we show that any $f \in \text{Fil}_k^{\text{W}}(\mathcal{MD})$ can be written as a polynomial in $[1]$. If we show that for a fixed l and $f \in \text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD})$ one can find $g_1 \in \text{Fil}_{k,l}^{\text{W,L}}(\mathfrak{qMZ})$ and $g_2, g_3 \in \text{Fil}_{k,l-1}^{\text{W,L}}(\mathcal{MD})$ such that f can be written as

$$f = g_1 + [1] \cdot g_2 + g_3, \tag{2.1}$$

then the claim follows directly by induction on l .

To show (2.1) it is clear that we can focus on the generators of \mathcal{MD} which we write as $f = [\{1\}^m, s_1, \dots, s_{l-m}]$, with $s_1 > 1$ and $k = m + s_1 + \dots + s_{l-m}$. By induction over m we prove that every element of such form can be written as in (2.1). For $m = 0$ it is $f \in \text{Fil}_k^{\text{W}}(\text{qMZ})$, i.e. $g_1 = f$ and $g_2 = g_3 = 0$. For the induction step we obtain by the quasi-shuffle product

$$m \cdot [\{1\}^m, s_1, \dots, s_{l-m}] = [1] \cdot [\{1\}^{m-1}, s_1, \dots, s_{l-m}] - g_3 \\ - \sum_{\substack{m_1 + \dots + m_i = m \\ m_j \geq 0, \forall j = 1 \dots i \\ m_1 < m}} [\{1\}^{m_1}, s_1, \{1\}^{m_2}, \dots, s_{l-m}, \{1\}^{m_i}].$$

with $g_3 \in \text{Fil}_{k, l-1}^{\text{W, L}}(\mathcal{MD})$. The elements in the sum start with at most $m - 1$ ones, so we obtain a representation in the form of (2.1) inductively.

- ii) We have to show that $[1]$ is algebraically independent over qMZ and therefore the representation of $f \in \mathcal{MD}$ in i) as a polynomial in $[1]$ with coefficients in qMZ is unique. From Proposition 6.4 we obtain that for $[s_1, \dots, s_l] \in \text{qMZ}$ with $s_1 + \dots + s_l = k$ we have for q close to 1 the approximations $[s_1, \dots, s_l] \approx \frac{1}{(1-q)^k}$ and from Remark 6.7 we know $[1] \approx \frac{-\log(1-q)}{1-q}$. Therefore the only polynomial in $\text{qMZ}[T]$, which has $[1]$ as one of its roots, is the constant polynomial 0.

□

Remark 2.15. It is clear that $[1]$ is an irreducible element in the ring \mathcal{MD} , thus it is clear that $\mathcal{MD}/([1] \cdot \mathcal{MD})$ is a domain. But the non-obvious fact is that this domain can be represented by qMZ .

At the end of this section we want to mention two other subalgebras of \mathcal{MD} . For this denote by $\mathcal{MD}^{\text{even}}$ the space spanned by 1 and all $[s_1, \dots, s_l]$ with s_j even for all $0 \leq j \leq l$ and by \mathcal{MD}^\sharp the space spanned by all by 1 and all $[s_1, \dots, s_l]$ with $s_j > 1$.

Proposition 2.16. $\mathcal{MD}^{\text{even}}$ and \mathcal{MD}^\sharp are subalgebras of \mathcal{MD} .

Proof. By the quasi-shuffle product formula Proposition 2.10 it is sufficient to show that for $1 \leq j \leq a$ the $\lambda_{a,b}^j \in \mathbb{Q}$ given by

$$\lambda_{a,b}^j = (-1)^{b-1} \binom{a+b-j-1}{a-j} \frac{B_{a+b-j}}{(a+b-j)!}$$

vanish for j odd if a and b are even to prove that $\mathcal{MD}^{\text{even}}$ is a subalgebra of \mathcal{MD} . But this follows directly by the fact that the B_k vanish for odd $k > 1$ and that the case $a + b - j = 1$ does not occur since $j \leq a$ and $b \geq 2$.

In order to prove that \mathcal{MD}^\sharp is a subalgebra of \mathcal{MD} we have to show that

$$\lambda_{a,b}^1 + \lambda_{b,a}^1 = ((-1)^{a-1} + (-1)^{b-1}) \binom{a+b-2}{a-1} \frac{B_{a+b-1}}{(a+b-1)!}$$

vanishes for $a, b > 1$. This term clearly vanishes when a and b have different parity. In the other case it is $B_{a+b-1} = 0$, because $a+b-1$ is odd and greater than 1. Hence it is $\lambda_{a,b}^1 + \lambda_{b,a}^1 = 0$, whenever $a, b > 1$. \square

The space \mathcal{MD}^\sharp is studied further in [BK], where the authors consider a connection of this space to other q -analogues of multiple zeta values.

3 A derivation and linear relations in \mathcal{MD}

Our strategy to prove Theorem 1.7 is to use generating series of brackets. This allows us to express the derivative in terms of elements in \mathcal{MD} . We make these calculations explicit in the case of first in the length 1 case and then for the length 2 case. Similar formulas for the general case are rather complicated.

Lemma 3.1. The generating series $T(X_1, \dots, X_l)$ of brackets of length l can be written as

$$T(X_1, \dots, X_l) = \sum_{s_1, \dots, s_l > 0} [s_1, \dots, s_l] X_1^{s_1-1} \dots X_l^{s_l-1} = \sum_{n_1, \dots, n_l > 0} \prod_{j=1}^l \frac{e^{n_j X_j} q^{n_1 + \dots + n_j}}{1 - q^{n_1 + \dots + n_j}}.$$

Proof. This can be seen by direct computation using the geometric series and the Taylor expansion of the exponential function:

$$\begin{aligned} \sum_{n_1, \dots, n_l > 0} \prod_{j=1}^l \frac{e^{n_j X_j} q^{n_1 + \dots + n_j}}{1 - q^{n_1 + \dots + n_j}} &= \sum_{n_1, \dots, n_l > 0} \prod_{j=1}^l e^{n_j X_j} \sum_{v_j > 0} q^{v_j(n_1 + \dots + n_j)} \\ &= \sum_{n_1, \dots, n_l > 0} \prod_{j=1}^l \sum_{k_j \geq 0} \frac{n_j^{k_j}}{k_j!} X_j^{k_j} \sum_{v_j > 0} q^{v_j(n_1 + \dots + n_j)} \\ &\stackrel{u_j = v_j + \dots + v_l}{=} \sum_{k_1, \dots, k_l \geq 0} \left(\sum_{\substack{u_1 > \dots > u_l > 0 \\ n_1, \dots, n_l > 0}} \frac{n_1^{k_1} \dots n_l^{k_l}}{k_1! \dots k_l!} q^{u_1 n_1 + \dots + u_l n_l} \right) X_1^{k_1} \dots X_l^{k_l} \\ &= \sum_{s_1, \dots, s_l > 0} [s_1, \dots, s_l] X_1^{s_1-1} \dots X_l^{s_l-1}. \end{aligned}$$

\square

We now study the derivative of brackets of length 1, much of the formulas presented for this purpose may implicitly found also in [GKZ]. In particular the next lemma is essentially a part of the calculation in the proof of Theorem 7 in [GKZ]. We give it nevertheless because it is a good preparation for the proof of our Theorem 1.7.

Lemma 3.2. i) The product of two generating functions of multiple divisor sums of length 1 is given by

$$T(X) \cdot T(Y) = T(X + Y, X) + T(X + Y, Y) - T(X + Y) + R_1(X, Y)$$

where

$$R_1(X, Y) = \sum_{n>0} e^{n(X+Y)} \frac{q^n}{(1-q^n)^2}.$$

ii) We have

$$\sum_{n>0} e^{nX} \frac{q^n}{(1-q^n)^2} = \sum_{k>0} \frac{d[k]}{k} X^k + [2].$$

In particular

$$R_1(X, Y) = \sum_{k>0} \frac{d[k]}{k} (X + Y)^k + [2].$$

Proof. i) Remember that the generating functions are given by

$$T(X) = \sum_{k>0} [k] X^{k-1} = \sum_{n>0} e^{nX} \frac{q^n}{1-q^n}$$

and

$$T(X, Y) = \sum_{s_1, s_2 > 0} [s_1, s_2] X^{s_1-1} Y^{s_2-1} = \sum_{n_1, n_2 > 0} e^{n_1 X + n_2 Y} \frac{q^{n_1}}{1-q^{n_1}} \frac{q^{n_2}}{1-q^{n_2}}.$$

With this in our hands we calculate

$$\begin{aligned} T(X)T(Y) &= \sum_{n_1, n_2 > 0} e^{n_1 X + n_2 Y} \frac{q^{n_1}}{1-q^{n_1}} \frac{q^{n_2}}{1-q^{n_2}} \\ &= \sum_{n_1 > n_2 > 0} \dots + \sum_{n_2 > n_1 > 0} \dots + \sum_{n_2 = n_1 > 0} \dots =: F_1 + F_2 + F_3. \end{aligned}$$

For these terms we get furthermore

$$\begin{aligned} F_1 &= \sum_{n_1 > n_2 > 0} e^{n_1 X + n_2 Y} \frac{q^{n_1}}{1-q^{n_1}} \frac{q^{n_2}}{1-q^{n_2}} \\ &\stackrel{n_1 = n_2 + n'_1}{=} \sum_{n'_1, n_2 > 0} e^{n'_1 X + n_2 (X+Y)} \frac{q^{n'_1 + n_2}}{1-q^{n'_1 + n_2}} \frac{q^{n_2}}{1-q^{n_2}} = T(X + Y, X) \end{aligned}$$

$$F_2 = \sum_{n_2 > n_1 > 0} e^{n_1 X + n_2 Y} \frac{q^{n_1}}{1 - q^{n_1}} \frac{q^{n_2}}{1 - q^{n_2}}$$

$$\stackrel{n_2 = n_1 + n'_2}{=} \sum_{n_1, n'_2 > 0} e^{n_1(X+Y) + n_2 Y} \frac{q^{n_1}}{1 - q^{n_1}} \frac{q^{n_1 + n'_2}}{1 - q^{n_1 + n'_2}} = T(X + Y, Y).$$

Using $\left(\frac{q^n}{1-q^n}\right)^2 = \frac{q^n}{(1-q^n)^2} - \frac{q^n}{1-q^n}$, we get for the last term

$$F_3 = \sum_{n_1 = n_2 > 0} e^{n_1(X+Y)} \left(\frac{q^{n_1}}{1 - q^{n_1}}\right)^2$$

$$= \sum_{n > 0} e^{n(X+Y)} \frac{q^n}{(1 - q^n)^2} - \sum_{n > 0} e^{n(X+Y)} \frac{q^n}{(1 - q^n)}$$

$$= R_1(X, Y) - T(X + Y).$$

ii) This can be seen by direct computation. First observe

$$dT(X) = \sum_{k > 0} d[k] X^{k-1} = d \sum_{n > 0} e^{nX} \frac{q^n}{1 - q^n} = \sum_{n > 0} n e^{nX} \frac{q^n}{(1 - q^n)^2}.$$

and then use this to evaluate

$$\sum_{k > 0} \frac{d[k]}{k} X^k = \sum_{k > 0} \int_0^X d[k] t^{k-1} dt$$

$$= \int_0^X dT(t) dt = \sum_{n > 0} \int_0^X n e^{nt} dt \frac{q^n}{(1 - q^n)^2}$$

$$= \sum_{n > 0} e^{nX} \frac{q^n}{(1 - q^n)^2} - \sum_{n > 0} \frac{q^n}{(1 - q^n)^2} = \sum_{n > 0} e^{nX} \frac{q^n}{(1 - q^n)^2} - [2].$$

□

We now want to give explicit expressions for the derivative of multiple divisor sums of length 1, which follow from the lemmas above:

Proposition 3.3. For s_1, s_2 with $s_1 + s_2 > 2$ and $s = s_1 + s_2 - 2$ we have the following expression for $d[s]$:

$$\binom{s}{s_1 - 1} \frac{d[s]}{s} = [s_1] \cdot [s_2] + \binom{s}{s_1 - 1} [s+1] - \sum_{a+b=s+2} \left(\binom{a-1}{s_1 - 1} + \binom{a-1}{s_2 - 1} \right) [a, b].$$

Proof. This is a direct consequence of Lemma 3.2 by considering the coefficient of $X^{s_1-1} Y^{s_2-1}$ in the equation

$$T(X) \cdot T(Y) = T(X + Y, X) + T(X + Y, Y) - T(X + Y) + \sum_{k > 0} \frac{d[k]}{k} (X + Y)^k + [2].$$

by using

$$\begin{aligned}
 T(X+Y, X) + T(X+Y, Y) &= \sum_{\substack{s_1, s_2 > 0 \\ a+b=s_1+s_2}} \left(\binom{a-1}{s_1-1} + \binom{a-1}{s_2-1} \right) [a, b] X^{s_1-1} Y^{s_2-1}, \\
 T(X+Y) &= \sum_{s_1, s_2 > 0} \left(\binom{s_1+s_2-2}{s_1-1} [s_1+s_2-1] \right) X^{s_1-1} Y^{s_2-1}, \\
 \sum_{k>0} \frac{d[k]}{k} (X+Y)^k &= \sum_{s_1, s_2 > 0} \left(\binom{s_1+s_2-2}{s_1-1} \frac{d[s_1+s_2-2]}{s_1+s_2-2} \right) X^{s_1-1} Y^{s_2-1}.
 \end{aligned}$$

□

Example 3.4. In the following formulas we used the explicit description for the product given in Proposition 2.8.

i) In the smallest case $s = 1$ there is just one choice given by $s_1 = 1, s_2 = 2$:

$$d[1] = [3] + \frac{1}{2}[2] - [2, 1].$$

ii) For $s = 2$ we can choose $s_1 = 1, s_2 = 3$ and $s_1 = s_2 = 2$ and therefore we get the two expressions:

$$\begin{aligned}
 d[2] &= 2[4] + [3] + \frac{1}{6}[2] - 2[2, 2] - 2[3, 1], \\
 d[2] &= [4] + 2[3] - \frac{1}{6}[2] - 4[3, 1],
 \end{aligned}$$

from which the first linear relation in weight 4 follows:

$$[4] = 2[2, 2] - 2[3, 1] + [3] - \frac{1}{3}[2].$$

iii) In the case $s = 3$ one again gets two expressions and therefore one relation.

iv) For $s = 4$ one has $s_1 = 1, s_2 = 5$ or $s_1 = 2, s_2 = 4$ and $s_1 = s_2 = 3$ which gives

$$\begin{aligned}
 d[4] &= 4[6] + 2[5] + \frac{1}{3}[4] - \frac{1}{180}[2] - 4[2, 4] - 4[3, 3] - 4[4, 2] - 4[5, 1], \\
 d[4] &= [6] + 4[5] - \frac{1}{12}[4] + \frac{1}{180}[2] - 2[3, 3] - 3[4, 2] - 8[5, 1], \\
 d[4] &= \frac{2}{3}[6] + 4[5] - \frac{1}{180}[2] - 4[4, 2] - 8[5, 1].
 \end{aligned}$$

From which the following two relations follow

$$\begin{aligned} 5[6] &= 3[5] - \frac{1}{2}[4] + 6[2, 4] + 6[3, 3] - 6[5, 1] \\ 3[6] &= 2[5] - \frac{5}{12}[4] + \frac{1}{90}[2] + 4[2, 4] + 2[3, 3] + [4, 2] - 4[5, 1]. \end{aligned}$$

Theorem 3.5. Suppose $k \geq 4$, then there are at least $\lfloor \frac{k}{2} \rfloor - 1$ linear relations in the generators of $\text{gr}_{k,2}^{\text{W,L}}(\text{qMZ})$.

Proof. It is clear that the expressions for $d[k-2]$ in Proposition 3.3 are symmetric in s_1 and s_2 . There are $\lfloor \frac{k}{2} \rfloor$ choices for s_1 and s_2 with $s_1 + s_2 = k$ and $s_1 \leq s_2$. For each such choice we get a different expression for $d[k-2]$, because for $s_1 \leq s_2$ it only contains the length 2 terms $[s_1 + 1, s_2 - 1], \dots, [s_1 + s_2 - 1, 1] \in \text{qMZ}$ with non vanishing coefficients. This can be seen if we rewrite the statement by using the stuffle product $[s_1] \cdot [s_2] = [s_1, s_2] + [s_2, s_1] + [s_1 \diamond s_2]$:

$$\begin{aligned} & \binom{k-2}{s_1-1} \frac{d[k-2]}{k-2} \\ &= [s_1 \diamond s_2] + \binom{k-2}{s_1-1} [k-1] - \sum_{\substack{a+b=k \\ a>s_1}} \left(\binom{a-1}{s_1-1} + \binom{a-1}{s_2-1} - \delta_{a,s_2} \right) [a, b]. \end{aligned}$$

By the same considerations as in proof of Theorem 2.13 we find that $[s_1 \diamond s_2] \in \text{qMZ}$. Therefore we get $\lfloor \frac{k}{2} \rfloor - 1$ relations. \square

We have checked that for $k \leq 20$ we get all relations in length two by the above method, cf. Theorem 5.5. This give some evidence for

Conjecture 3.6. For all weights $k \geq 4$ the number of linear relations in the generators of $\text{gr}_{k,2}^{\text{W,L}} \text{qMZ}$ equals $\lfloor \frac{k}{2} \rfloor - 1$.

Now we want to consider the derivative in the length two case.

Lemma 3.7. The product of two generating functions of multiple divisor sums of length 1 and 2 is given by

$$\begin{aligned} T(X) \cdot T(Y, Z) &= T(X+Y, Y, Z) + T(X+Y, X+Z, Z) + T(X+Y, X+Z, X) \\ &\quad - T(X+Y, Z) - T(X+Y, X+Z) + R_2(X, Y, Z), \end{aligned}$$

where

$$\begin{aligned} R_2(X, Y, Z) &= \sum_{n_1, n_2 > 0} e^{n_1(X+Y)+n_2Z} \frac{q^{n_1}}{(1-q^{n_1})^2} \frac{q^{n_1+n_2}}{1-q^{n_1+n_2}} \\ &\quad + \sum_{n_1, n_2 > 0} e^{n_1(X+Y)+n_2(X+Z)} \frac{q^{n_1}}{1-q^{n_1}} \frac{q^{n_1+n_2}}{(1-q^{n_1+n_2})^2} \end{aligned}$$

Proof. i) We again split the sum into different parts as in the case for $T(X)T(Y)$:

$$\begin{aligned} T(X) \cdot T(Y, Z) &= \sum_{n_1, n_2, n_3 > 0} e^{n_1 X + n_2 Y + n_3 Z} \frac{q^{n_1}}{1 - q^{n_1}} \frac{q^{n_2}}{1 - q^{n_2}} \frac{q^{n_2 + n_3}}{1 - q^{n_2 + n_3}} \\ &= \sum_{n_2 > n_1} \cdots + \sum_{n_1 > n_2 + n_3} \cdots + \sum_{n_2 + n_3 > n_1 > n_2} \cdots + \sum_{n_1 = n_2} \cdots + \sum_{n_1 = n_2 + n_3} \cdots \\ &=: F_1 + F_2 + F_3 + F_4 + F_5. \end{aligned}$$

The proof of $F_1 + F_2 + F_3 = T(X + Y, Y, Z) + T(X + Y, X + Y, Z) + T(X + Y, X + Y, X)$ is similar to the calculation in the lemma above and we leave it out here. The evaluation of F_4 and F_5 are similar and we therefore just illustrate the F_4 case:

$$\begin{aligned} F_4 &= \sum_{n_1 = n_2, n_3 > 0} e^{n_1(X+Y) + n_3 Z} \left(\frac{q^{n_1}}{1 - q^{n_1}} \right)^2 \frac{q^{n_1 + n_3}}{1 - q^{n_1 + n_3}}, \\ &= \sum_{n_1 = n_2, n_3 > 0} e^{n_1(X+Y) + n_3 Z} \left(\frac{q^{n_1}}{(1 - q^{n_1})^2} - \frac{q^{n_1}}{1 - q^{n_1}} \right) \frac{q^{n_1 + n_3}}{1 - q^{n_1 + n_3}}, \\ &= \sum_{n_1, n_3 > 0} e^{n_1(X+Y) + n_3 Z} \frac{q^{n_1}}{(1 - q^{n_1})^2} \frac{q^{n_1 + n_3}}{1 - q^{n_1 + n_3}} - T(X + Y, Z). \end{aligned}$$

□

Definition 3.8. We define the operator $D(f)$ on functions in X by

$$D(f) = \left(\frac{\partial}{\partial X} f \right) \Big|_{X=0}.$$

Observe that $D(R_1(X, Y)) = dT(Y)$ and for the length 2 it holds

Lemma 3.9. We have

$$D(R_2(X, Y, Z)) = dT(Y, Z).$$

Proof. For the two summands of $R_2(X, Y, Z)$ one gets

$$\begin{aligned} D \left(\sum_{n_1, n_2 > 0} e^{n_1(X+Y) + n_2 Z} \frac{q^{n_1}}{(1 - q^{n_1})^2} \frac{q^{n_1 + n_2}}{1 - q^{n_1 + n_2}} \right) &= \\ &= \sum_{n_1, n_2 > 0} n_1 e^{n_1 Y + n_2 Z} \frac{q^{n_1}}{(1 - q^{n_1})^2} \frac{q^{n_1 + n_2}}{1 - q^{n_1 + n_2}}, \\ D \left(\sum_{n_1, n_2 > 0} e^{n_1(X+Y) + n_2(X+Z)} \frac{q^{n_1}}{1 - q^{n_1}} \frac{q^{n_1 + n_2}}{(1 - q^{n_1 + n_2})^2} \right) &= \\ &= \sum_{n_1, n_2 > 0} (n_1 + n_2) e^{n_1 Y + n_2 Z} \frac{q^{n_1}}{1 - q^{n_1}} \frac{q^{n_1 + n_2}}{(1 - q^{n_1 + n_2})^2}. \end{aligned}$$

Adding these two terms one obtains $dT(Y, Z)$, because with $d \frac{q^n}{1-q^n} = \frac{n \cdot q^n}{(1-q^n)^2}$ and the product formula we obtain

$$\begin{aligned} dT(Y, Z) &= d \sum_{n_1, n_2 > 0} e^{n_1 Y + n_2 Z} \frac{q^{n_1}}{1-q^{n_1}} \frac{q^{n_1+n_2}}{1-q^{n_1+n_2}} = \\ &\sum_{n_1, n_2 > 0} \left(n_1 e^{n_1 Y + n_2 Z} \frac{q^{n_1}}{(1-q^{n_1})^2} \frac{q^{n_1+n_2}}{1-q^{n_1+n_2}} + (n_1 + n_2) e^{n_1 Y + n_2 Z} \frac{q^{n_1}}{1-q^{n_1}} \frac{q^{n_1+n_2}}{(1-q^{n_1+n_2})^2} \right) \end{aligned}$$

□

Proposition 3.10. The derivative of $[s_1, s_2]$ can be written as

$$\begin{aligned} d[s_1, s_2] &= [2] \cdot [s_1, s_2] - s_1[s_1 + 1, s_2, 1] - s_2[s_1, s_2 + 1, 1] - [s_1, s_2, 2] \\ &- \left(\sum_{a+b=s_1+2} (a-1)[a, b, s_2] + \sum_{a+b=s_2+1} s_1[s_1 + 1, a, b] + \sum_{a+b=s_2+2} (a-1)[s_1, a, b] \right) \\ &+ 2s_1[s_1 + 1, s_2] + s_2[s_1, s_2 + 1]. \end{aligned}$$

Proof. This follows directly from Lemma 3.7 by applying the operator

$$D(f) = \left(\frac{d}{dX} f \right) \Big|_{X=0}$$

on both sides of the equation. It is straightforward to calculate $D(T(\dots, \dots))$ for the various generating series $T(\dots, \dots)$ in Lemma 3.7, e.g., the lefthand side becomes $[2] \cdot T(Y, Z)$. By means of Lemma 3.9 the claim follows easily by collecting all the terms. □

Example 3.11. i) For $s_1 = s_2 = 1$ Proposition 3.10 gives the representation of $d[1, 1]$ already mentioned above in (1.8):

$$d[1, 1] = [3, 1] + [1, 3] + \frac{3}{2}[2, 1] + \frac{1}{2}[1, 2] - 2[2, 1, 1] - [1, 2, 1];$$

here we used the quasi-shuffle product

$$[2] \cdot [1, 1] = [3, 1] + [1, 3] + [2, 1, 1] + [1, 2, 1] + [1, 1, 2] - \frac{1}{2}[2, 1] - \frac{1}{2}[1, 2].$$

ii) For $s_1 = 1, s_2 = 2$ the corollary gives

$$d[1, 2] = -\frac{1}{6}[1, 2] + 2[1, 3] + [1, 4] + \frac{3}{2}[2, 2] + [3, 2] - 4[1, 3, 1] - [2, 1, 2] - 2[2, 2, 1].$$

iii) For $s_1 = 1, s_2 = 2$ the corollary gives

$$d[2, 1] = -\frac{1}{6}[2, 1] + \frac{1}{2}[2, 2] + [2, 3] + 4[3, 1] + [4, 1] - [2, 2, 1] - 6[3, 1, 1].$$

iv) The case $s_1 = s_2 = 2$ is given by

$$d[2, 2] = -\frac{1}{3}[2, 2] + 2[2, 3] + [2, 4] + 4[3, 2] + [4, 2] - 4[2, 3, 1] - 4[3, 1, 2] - 4[3, 2, 1].$$

At this point we like to indicate that the Leibniz rule is another source of linear relations in \mathcal{MD} .

Example 3.12. i) By means of the Leibniz rule and the quasi-shuffle product we have

$$d[1] \cdot [2] + [1] \cdot d[2] = d([1] \cdot [2]) = d\left([1, 2] + [2, 1] + [3] - \frac{1}{2}[2]\right).$$

Evaluating both sides separately we deduce the following linear relation in length 3

$$\begin{aligned} [5] &= 2[3, 1, 1] - [2, 2, 1] + [2, 3] + 2[3, 2] - [4, 1] \\ &\quad + \frac{1}{2}[4] + \frac{1}{2}[2, 2] - 2[3, 1] + \frac{1}{6}[2, 1] - \frac{1}{12}[2] + \frac{1}{12}[3]. \end{aligned} \quad (3.1)$$

ii) Using the same argument for $[1] \cdot [3]$ we have

$$d[1] \cdot [3] + [1] \cdot d[3] = d([1][3]) = d\left([1, 3] + [3, 1] + [4] + \frac{1}{12}[2] - \frac{1}{2}[3]\right)$$

from which the following relation in weight 6 follows

$$\begin{aligned} [6] &= \frac{1}{120}[2] - \frac{1}{24}[3] + \frac{1}{2}[5] + \frac{1}{4}[2, 2] - [2, 2, 2] + \frac{1}{2}[2, 3] - [2, 3, 1] \\ &\quad + [2, 4] + \frac{1}{12}[3, 1] + 2[3, 1, 2] - [3, 2] - 3[4, 1] + 3[4, 1, 1] + 5[4, 2] - [5, 1]. \end{aligned}$$

Theorem 3.13. i) There is a linear relation in the generators of $\text{gr}_{5,3}^{\text{W,L}}(\mathcal{qMZ})$.

ii) There are at least 3 linear relations in the generators of $\text{gr}_{6,3}^{\text{W,L}}(\mathcal{qMZ})$.

Proof. i) From Example 3.12 i) we deduce the relation

$$0 \equiv 2[3, 1, 1] - [2, 2, 1]$$

in $\text{gr}_{5,3}^{\text{W,L}}(\mathcal{qMZ})$.

ii) From Example 3.12 ii) we deduce the relation

$$0 \equiv 2[3, 1, 2] + 3[4, 1, 1]$$

in $\text{gr}_{6,3}^{\text{W,L}}(\mathfrak{qM}\mathcal{Z})$ and from Example 1.12 we deduce that

$$\begin{aligned} 0 &\equiv 3[2, 2, 2] - [3, 1, 2] - [2, 3, 1] - [3, 2, 1] \\ 0 &\equiv -4[2, 3, 1] - 4[3, 1, 2] - [3, 2, 1] + 9[4, 1, 1] \end{aligned}$$

□

We finally want to prove that the map d is a derivation for arbitrary length using the same combinatorial arguments as in the length one and two cases but without calculating explicit representations for $d[s_1, \dots, s_l]$.

Proof. (of Theorem 1.7) To prove this statement we are going to use the same combinatorial arguments as in the Lemma 3.7, Lemma 3.9 and Proposition 3.10 in a general way which means that we have

$$\begin{aligned} T(X) \cdot T(Y_1, \dots, Y_l) &= \sum_{m, n_1, \dots, n_l > 0} e^{mX + n_1 Y_1 + \dots + n_l Y_l} \frac{q^m}{1 - q^m} \frac{q^{n_1}}{1 - q^{n_1}} \cdots \frac{q^{n_1 + \dots + n_l}}{1 - q^{n_1 + \dots + n_l}} \\ &= T(X + Y_1, \dots, X + Y_l, X) + \sum_{j=1}^l T(X + Y_1, \dots, X + Y_j, Y_j, \dots, Y_l) \\ &\quad + R_l - \sum_{j=1}^l T(X + Y_1, \dots, X + Y_j, Y_{j+1}, \dots, Y_l), \end{aligned} \tag{3.2}$$

where

$$R_l = \sum_{j=1}^l \left(\sum_{n_1, \dots, n_l > 0} e^{n_1(X+Y_1) + \dots + n_j(X+Y_j) + n_{j+1}Y_{j+1} + \dots + n_l Y_l} \prod_{i=1}^l \frac{q^{n_1 + \dots + n_i}}{(1 + q^{n_1 + \dots + n_i})^{\delta_{i,j+1}}} \right).$$

This can be seen by splitting up the sum in the same way as above. The first line comes from the parts where one sums over the ordered pairs $n_1 + \dots + n_{j-1} < m < n_1 + \dots + n_j$ for $j = 1, \dots, l$ and $n_1 + \dots + n_l < m$. Setting $m = n_1 + \dots + n_{j-1} + m'$ and $n_j = m' + n'_j$ for these terms it is easy to see that one gets the sum over $m', n_1, \dots, n'_j, \dots, n_l$ which then gives $T(X + Y_1, \dots, X + Y_j, Y_j, \dots, Y_l)$.

The second line arises from the sum over $m = n_1 + \dots + n_j$. In this case one again uses the identity

$$\left(\frac{q^n}{1 - q^n} \right)^2 = \frac{q^n}{(1 - q^n)^2} - \frac{q^n}{1 - q^n}$$

from which the rest follows easily.

Letting the operator $D(f) = \left(\frac{d}{dX}f\right) \Big|_{X=0}$ act on this it is easy to see that the last term then becomes

$$D(R_l) = \sum_{j=1}^l \left(\sum_{n_1, \dots, n_l > 0} (n_1 + \dots + n_j) e^{n_1 Y_1 + \dots + n_l Y_l} \prod_{i=1}^l \frac{q^{n_1 + \dots + n_i}}{(1 + q^{n_1 + \dots + n_i})^{\delta_{i,j+1}}} \right)$$

and this is exactly $dT(Y_1, \dots, Y_l)$ which can be seen by induction on l and the product formula. The product on the left becomes $[2]T(Y_1, \dots, Y_l)$ and the remaining terms on the right all have elements in $\text{Fil}_{k+2, l+1}^{\text{W,L}}(\mathcal{MD})$ as their coefficients and therefore the statement follows. \square

Proposition 3.14. The space qMZ is closed under d .

Proof. This follows directly by the proof of Theorem 1.7 since in the formula for $dT(Y_1, \dots, Y_l)$, which one obtains by applying D to equation (3.2), it is easy to see that the coefficients of the monomials which contains a Y_1 are all in qMZ . \square

Remark 3.15. We didn't give an explicit formula for the derivative of brackets of length l , since a general formula seems to be confusing. But for a specific bracket one can get its derivative by applying first the operator D to the equation (3.2) and then collecting the corresponding coefficients. For example for $l = 3$ one can deduce

$$\begin{aligned} d[2, 1, 1] &= -\frac{1}{6}[2, 1, 1] + \frac{1}{2}[2, 1, 2] - [2, 1, 2, 1] + [2, 1, 3] + \frac{3}{2}[2, 2, 1] \\ &\quad - 2[2, 2, 1, 1] + [2, 3, 1] + 6[3, 1, 1] - 8[3, 1, 1, 1] + [4, 1, 1]. \end{aligned}$$

Remark 3.16. Changing the perspective we can view Theorem 1.7) and its special cases Lemma 3.7, Lemma 3.9 and Proposition 3.10 as results, which express the failure of the shuffle relation for $[s] \cdot [s_1, \dots, s_l]$ in terms of multiple divisor functions of lower weight and length and derivatives. An optimistic guess is that this is also the case for more complicated products. We want to come back to this in [BBK].

4 The subalgebra of (quasi-)modular forms

We call

$$G_k = \frac{\zeta(k)}{(2\pi i)^k} + \frac{1}{(k-1)!} \sum_{n>0} \sigma_{k-1}(n) q^n = \frac{\zeta(k)}{(2\pi i)^k} + [k].$$

the Eisenstein series of weight k . For even $k = 2n$ due to Eulers theorem we have in addition

$$\zeta(2n) = \frac{(-1)^{n-1} B_{2n} (2\pi)^{2n}}{2(2n)!}$$

and therefore

$$G_{2n} = -\frac{1}{2} \frac{B_{2n}}{(2n)!} + [2n] \in \text{Fil}_{2n}^{\text{W}}(\mathcal{MD}),$$

for example

$$G_2 = -\frac{1}{24} + [2], \quad G_4 = \frac{1}{1440} + [4], \quad G_6 = -\frac{1}{60480} + [6].$$

Proposition 4.1. i) The ring of modular forms $M(\Gamma_1)$ for $\Gamma_1 = SL_2(\mathbb{Z})$ and the ring of quasi-modular forms $\widetilde{M}(\Gamma_1)$ are graded subalgebras of \mathcal{MD} .

ii) The \mathbb{Q} -algebra of quasi-modular forms $\widetilde{M}_k(\Gamma_1)$ is closed under the derivation d and therefore it is a subalgebra of the graded differential algebra (\mathcal{MD}, d) .

iii) We have the following inclusions of \mathbb{Q} -algebras

$$M_k(\Gamma_1) \subset \widetilde{M}(\Gamma_1) \subset \mathcal{MD}^{\text{even}} \subset \mathcal{MD}^{\sharp} \subset \mathfrak{q}\mathcal{MZ} \subset \mathcal{MD}.$$

Proof. Let $M_k(\Gamma_1)$ (resp. $\widetilde{M}_k(\Gamma_1)$) be the space of (quasi-)modular forms of weight k for Γ_1 . Then the first claim follows directly from the well-known facts

$$\begin{aligned} M(\Gamma_1) &= \bigoplus_{k>1} M(\Gamma_1)_k = \mathbb{Q}[G_4, G_6] \\ \widetilde{M}(\Gamma_1) &= \bigoplus_{k>1} \widetilde{M}(\Gamma_1)_k = \mathbb{Q}[G_2, G_4, G_6]. \end{aligned}$$

The second claim is a well known fact in the theory of quasi-modular forms and a proof can be found in [Za2] p. 49. It suffices to show that the derivatives of the generators are given by

$$\begin{aligned} dG_2 &= d[2] = 5G_4 - 2G_2^2, & dG_4 &= 15G_6 - 8G_2G_4, \\ dG_6 &= 20G_8 - 12G_2G_6 = \frac{120}{7}G_4^2 - 12G_2G_6. \end{aligned}$$

The last statement follows immediately by i) and the results before. \square

Remark 4.2. The above formulas for $d[2]$, $d[4]$ and $d[6]$ can also be proven with Proposition 3.3.

Example 4.3. The theory of modular forms yield linear relations in \mathcal{MD} . We indicate here how to derive such a relation in weight 8. It is a well-known fact from the theory of modular forms that $G_4^2 = \frac{7}{6}G_8$ because the space of weight 8 modular forms is one dimensional. We therefore have

$$\frac{1}{2073600} + \frac{1}{720}[4] + [4] \cdot [4] = \left(\frac{1}{1440} + [4] \right)^2 = \frac{1}{2073600} + \frac{7}{6}[8].$$

Using the quasi-shuffle product from Proposition 2.6 we get

$$[4] \cdot [4] = 2[4, 4] + [8] + \frac{1}{360}[4] - \frac{1}{1512}[2],$$

which then gives the following relation in weight 8:

$$[8] = \frac{1}{40}[4] - \frac{1}{252}[2] + 12[4, 4].$$

It is well known that the weight is additive for multiplication of modular forms. The above relation shows that the length is not additive with respect to the multiplication of modular forms.

Proposition 4.4. The algebra of modular forms is graded with respect to the weight and filtered with respect to the length. We have

$$\sum_k \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}} M(\Gamma_1) x^k y^l = 1 + \frac{x^4}{1-x^2} y + \frac{x^{12}}{(1-x^4)(1-x^6)} y^2,$$

in particular

$$\sum_k \dim_{\mathbb{Q}} M_k(\Gamma_1) x^k = \frac{1}{(1-x^4)(1-x^6)}.$$

Proof. For each k there is an Eisenstein series G_k and this is the only element of length 1 in $M_k(\Gamma_1)$. Now the first statement follows immediately from the fact that the polynomials $G_a G_b$ with $a + b = k$ generate $M_k(\Gamma_1)$ as a vector space [Za1]. Setting y in the first formula we see again that the modular forms G_4 and G_6 generate $M(\Gamma_1)$ as an algebra. \square

Notice that because of Theorem 1.6 we know all relations in $\text{Fil}_{8,2}^{\text{W,L}}(\mathcal{MD})$ and therefore we could give a purely algebraic proof the relation $G_4^2 = \frac{7}{6}G_8$ without using the theory of modular forms, which relies on complex analysis. Moreover, again using Theorem 1.6, we can prove in $\text{Fil}_{12}^{\text{W}}(\mathcal{MD})$ new identities for the cusp form $\Delta = \sum_{n>0} \tau(n)q^n$.

Proposition 4.5. For $(a, b) \in \{(2, 4), (4, 6), (6, 8), (8, 10), (10, 11), (11, 12)\}$ the cusp form $\Delta \in S_{12}$ can be uniquely written as

$$\Delta = \frac{2^b + 50}{2^b - 2^a} \cdot [a] + \frac{2^a + 50}{2^a - 2^b} \cdot [b] + \sum_{m+n=12} d_{m,n} \cdot [m, n],$$

where $d_{m,n} \in \mathbb{Q}$. Moreover, any other representation of Δ in $\text{Fil}_{12,2}^{\text{W,L}}(\mathcal{MD})$ is a linear combination of these six representations.

Proof. By Theorem 1.6 we just have to solve systems of linear equations coming from the coefficients of the brackets in question. Using the relations coming from Proposition 3.3 this can be made very efficient with the computer. \square

Taking a suitable linear combination of the identities in Proposition 4.5 we get the representation (1.13) of Δ given in the introduction.

Remark 4.6. At the end of this section we just want to give a short remark concerning the arithmetical aspect of the relations in Proposition 4.5 on which we don't want to focus in detail in these notes. Formulas like the ones above give several representation of the Fourier coefficients of cusp forms in terms of multiple divisor sums. One can also see the well-known congruence $\tau(n) \equiv \sigma_{11}(n) \pmod{691}$ and it is easy to derive a lot of other congruences involving $\tau(n)$ and the brackets out of such relations.

5 Experiments and conjectures: dimensions

In this section we present data of some computer calculations regarding the number of linear independent brackets with length and weight smaller or equal to 15. In some cases we can prove these bounds to be sharp. Based on these experiments, we make a conjecture on the dimension of the graded pieces of $\mathfrak{qM}\mathcal{Z}$ and therefore also for \mathcal{MD} . We first recall our results on the algebraic structure of \mathcal{MD} and $\mathfrak{qM}\mathcal{Z}$, where $\mathfrak{qM}\mathcal{Z}$ is the sub algebra of \mathcal{MD} generated by admissible brackets. Both are a bi-filtered algebras with respect to the filtration $\text{Fil}_\bullet^{\mathbf{W}}$ given by the weight and the filtration $\text{Fil}_\bullet^{\mathbf{L}}$ given by the length. Therefore as vector spaces we have

$$\mathcal{MD} \cong \bigoplus_k \text{gr}_k^{\mathbf{W}}(\mathcal{MD}) \cong \bigoplus_k \bigoplus_{l \leq k} \text{gr}_{k,l}^{\mathbf{W},\mathbf{L}}(\mathcal{MD}) \quad (5.1)$$

$$\mathfrak{qM}\mathcal{Z} \cong \bigoplus_k \text{gr}_k^{\mathbf{W}}(\mathfrak{qM}\mathcal{Z}) \cong \bigoplus_k \bigoplus_{l \leq k-1} \text{gr}_{k,l}^{\mathbf{W},\mathbf{L}}(\mathfrak{qM}\mathcal{Z}). \quad (5.2)$$

Proposition 5.1. In the direct sums in (5.1) and (5.2) each summand is a finite dimensional vector space. In particular, we have

$$\dim_{\mathbb{Q}} \text{gr}_{k,l}^{\mathbf{W},\mathbf{L}}(\mathcal{MD}) \leq \binom{k-1}{l-1}, \quad \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\mathbf{W},\mathbf{L}}(\mathfrak{qM}\mathcal{Z}) \leq \binom{k-2}{l-1}.$$

Proof. Let $b(k, l)$ denote the number of brackets $[s_1, \dots, s_l]$ of weight k and length l , i.e. $s_1 + \dots + s_l = k$ and let $a(k, l)$ denote the number of admissible brackets of this type, i.e. $s_1 + \dots + s_l = k$ with $s_1 > 1$. It suffices to show

$$b(k, l) = \binom{k-1}{l-1}, \quad a(k, l) = \binom{k-2}{l-1}. \quad (5.3)$$

Now, if we write $k = 1 + \dots + 1$, then these formulas are an easy combinatorial fact, which can be seen by counting the possible ways of replacing $l - 1$ of $k - 1$ plus symbols by a semi-column and then interpreting the remaining sums as tuples (s_1, \dots, s_l) (resp. $k - 2$ since we can't replace the first plus symbol). \square

Definition 5.2. We define

$$d'(k, l) = \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\text{qMZ}).$$

The next proposition shows that, in order to understand the dimensions of the various subspaces of qMZ as well as of \mathcal{MD} , which are induced by the filtration given by weight or length, it suffices to understand $d'(k, l)$.

Proposition 5.3. We have for qMZ the identities

$$\begin{aligned} \dim_{\mathbb{Q}} \text{gr}_k^{\text{W}}(\text{qMZ}) &= \sum_{i=0}^k d'(k, i) \\ \dim_{\mathbb{Q}} \text{Fil}_k^{\text{W}}(\text{qMZ}) &= \sum_{j=0}^k \sum_{i=0}^j d'(j, i) \\ \dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\text{qMZ}) &= \sum_{j=0}^k \sum_{i=0}^l d'(j, i) \end{aligned}$$

and for \mathcal{MD} we have

$$\begin{aligned} \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\mathcal{MD}) &= \sum_{j=0}^k d'(k-j, l-j) \\ \dim_{\mathbb{Q}} \text{gr}_k^{\text{W}}(\mathcal{MD}) &= \dim_{\mathbb{Q}} \text{Fil}_k^{\text{W}}(\text{qMZ}) = \sum_{l=0}^k \sum_{j=0}^k d'(k-j, l-j) \\ \dim_{\mathbb{Q}} \text{Fil}_k^{\text{W}}(\mathcal{MD}) &= \sum_{j=0}^k \sum_{i=0}^k \sum_{r=0}^j d'(j-r, i-r) \\ \dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\mathcal{MD}) &= \sum_{j=0}^k \sum_{i=0}^l \sum_{r=0}^j d'(j-r, i-r) \end{aligned}$$

Proof. If V is a vector space with filtration F_{\bullet} such that

$$0 = F_0(V) \subseteq F_1(V) \subseteq \dots \subseteq F_k(V) \subseteq \dots \subseteq V,$$

then $F_k(V) \cong \bigoplus_{j \leq k} \text{gr}_j^{\text{F}}(V)$. We further know that

$$\mathcal{MD} \cong \text{qMZ}[[1]],$$

hence modulo $\text{Fil}_{k,l-1}^{\text{W,L}}(\mathcal{M}\mathcal{D})$ and $\text{Fil}_{k-1,l}^{\text{W,L}}(\mathcal{M}\mathcal{D})$ we have

$$\text{gr}_{k,l}^{\text{W,L}}(\mathcal{M}\mathcal{D}) \equiv \sum_{i=0}^k \text{gr}_{k-i,l-i}^{\text{W,L}}(\text{q}\mathcal{M}\mathcal{Z})[1]^i.$$

Now the claim follows by the properties of the product. \square

Theorem 5.4. We have the following results for $\dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\text{q}\mathcal{M}\mathcal{Z})$

$k \setminus l$	0	1	2	3	4	5	6	7	8	9	10	11
0	1											
1	1	1										
2	1	2	2									
3	1	3	4	4								
4	1	4	6	7	7							
5	1	5	9	12	13	13						
6	1	6	12	18	22	23	23					
7	1	7	16	26	35	40	41	41				
8	1	8	20	36	53	66	72	73	73			
9	1	9	25	48	76	103	121	128	129	129		
10	1	10	30	63	107	155	196	220	228	229	229	
11	1	11	36	80	145	225	304	364	395	404	405	405
12	1	12	42	100	193	317	456	?	?	?	?	?
13	1	13	49	123	251	?	?	?	?	?	?	?
14	1	14	56	150	321	?	?	?	?	?	?	?
15	1	15	64	179	?	?	?	?	?	?	?	?

Table 2: $\dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\text{q}\mathcal{M}\mathcal{Z})$: **proven exact**, **proven lower bounds**.

Proof. We first explain how we obtain lower bounds with the help of a computer, then we give an upper bounds by listing enough relations.

Lower bounds:

We calculated with the help of a computer a reasonable number of the coefficients for each of the brackets in $\text{Fil}_{k,l}^{\text{W,L}}(\text{q}\mathcal{M}\mathcal{Z})$. Now the rank of the matrix whose rows are the coefficients gives us for $\dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\text{q}\mathcal{M}\mathcal{Z})$ a lower bound. Since we work only with a finite number of columns, it may happen that we can't distinguish

linear independent elements. The result of our computer calculations is that all the entries³ in the table of Theorem 5.4 are lower bounds.

For example in the case of $\text{Fil}_{4,3}^{\text{W,L}}(\text{qMZ})$ we checked that the following matrix

$$\begin{pmatrix} 1 & 3 & 4 & 7 & 6 & 12 & 8 & 15 \\ \frac{1}{2} & \frac{5}{2} & 5 & \frac{21}{2} & 13 & 25 & 25 & \frac{85}{2} \\ \frac{1}{6} & \frac{3}{2} & \frac{14}{3} & \frac{73}{6} & 21 & 42 & \frac{172}{3} & \frac{195}{2} \\ 0 & 0 & 1 & 2 & 6 & 7 & 15 & 18 \\ 0 & 0 & 1 & 3 & 9 & 15 & 30 & 45 \\ 0 & 0 & \frac{1}{2} & 1 & 4 & \frac{9}{2} & \frac{25}{2} & 15 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 5 \end{pmatrix},$$

whose rows are the first 8 coefficients of the 7 brackets

$$[2], [3], [4], [2, 1], [2, 2], [3, 1], [2, 1, 1]$$

has rank 6. Thus there are at least 7 (including the constant) linear independent elements in $\text{Fil}_{4,3}^{\text{W,L}}(\text{qMZ})$ and therefore $\dim_{\mathbb{Q}} \text{Fil}_{4,3}^{\text{W,L}}(\text{qMZ}) \geq 7$.

Upper bounds:

Because of the identity

$$\dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\text{qMZ}) = \sum_{i \leq k, j \leq l} \dim_{\mathbb{Q}} \text{gr}_{i,j}^{\text{W,L}}(\text{qMZ})$$

it suffices to give upper bounds for $\dim_{\mathbb{Q}} \text{gr}_{i,j}^{\text{W,L}}(\text{qMZ})$. We use the bounds given by $a(k, l)$ minus the number of known relations between the generators. There is at least no relations in the generators of $\text{gr}_{k,1}^{\text{W,L}}(\text{qMZ})$, in fact $[k]$ is a generator. In $\text{gr}_{k,2}^{\text{W,L}}(\text{qMZ})$ we know by Theorem 3.5 that there are at least $\left\lfloor \frac{(k-2)}{2} \right\rfloor$ relations in between generators. In addition we know by Theorem 3.13 the number of relations in length 3 for the weights 5 and 6. Now it is easily checked that the lower and upper bounds coincide for the black marked entries in the table and hence the theorem is proven. For example in the case of $\text{Fil}_{4,3}^{\text{W,L}}(\text{qMZ})$ we have that

$$\begin{aligned} \dim_{\mathbb{Q}} \text{Fil}_{4,3}^{\text{W,L}}(\text{qMZ}) &\leq \sum_{0 \leq k \leq 4} \sum_{0 \leq l \leq 3} \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\text{qMZ}) \\ &= 1 + \sum_{2 \leq k \leq 4} (1 - 0) + \sum_{3 \leq k \leq 4} \left(\binom{k-2}{1} - \left\lfloor \frac{(k-2)}{2} \right\rfloor \right) + 1 - 0 \\ &= 1 + 3 + 2 + 1 = 7. \end{aligned}$$

³ The total running time on a standard PC for each entry was less then 24 hours. We point to the fact, that refinements of our code may give some more entries in the table.

□

Unfortunately there is no direct way to get the dimension of $\text{gr}_{k,l}^{\text{W,L}}(\mathfrak{q}\mathcal{M}\mathcal{Z})$ with the help of a computer. However we can deduce the following conditional result.

Theorem 5.5. i) We have the following results for $d'(k,l) = \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\mathfrak{q}\mathcal{M}\mathcal{Z})$

$k \setminus l$	0	1	2	3	4	5	6	7	8	9	10	11
0	1	0										
1	0	0										
2	0	1	0									
3	0	1	1	0								
4	0	1	1	1	0							
5	0	1	2	2	1	0						
6	0	1	2	3	3	1	0					
7	0	1	3	4	5	4	1	0				
8	0	1	3	6	8	8	5	1	0			
9	0	1	4	7	11	14	12	6	1	0		
10	0	1	4	10	16	21	23	17	7	1	0	
11	0	1	5	11	21	32	38	36	23	8	1	0
12	0	1	5	14	28	44	60	?	?	30	9	1
13	0	1	6	16	35	?	?	?	?	?	38	10
14	0	1	6	20	43	?	?	?	?	?	?	47
15	0	1	7	21	?	?	?	?	?	?	?	?

Table 3: $\dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\mathfrak{q}\mathcal{M}\mathcal{Z})$: **proven**, **conjectured**.

ii) We have the following results for the number of relations in $\dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\mathfrak{q}\mathcal{M}\mathcal{Z})$

$k \setminus l$	1	2	3	4	5	6	7	8	9	10
1										
2	0									
3	0	0								
4	0	1	0							
5	0	1	1	0						
6	0	2	3	1	0					
7	0	2	6	5	1	0				
8	0	3	9	12	7	1	0			
9	0	3	14	24	21	9	1	0		
10	0	4	18	40	49	33	11	1	0	
11	0	4	25	63	?	?	?	13	1	0
12	0	5	36	16	?	?	?	?	15	1
13	0	5	?	?	?	?	?	?	?	17
14	0	6	?	?	?	?	?	?	?	?
15	0	6	?	?	?	?	?	?	?	?

Table 4: Relations in $\dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\text{qMZ})$: **proven**, **conjectured**.

Proof. i) If the dimensions of $\text{Fil}_{k,l}^{\text{W,L}}(\text{qMZ})$ are given, then

$$\begin{aligned} \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\text{qMZ}) &= \dim_{\mathbb{Q}} \text{Fil}_{k,l}^{\text{W,L}}(\text{qMZ}) - \dim_{\mathbb{Q}} \text{Fil}_{k-1,l}^{\text{W,L}}(\text{qMZ}) \\ &\quad - \dim_{\mathbb{Q}} \text{Fil}_{k,l-1}^{\text{W,L}}(\text{qMZ}) + \dim_{\mathbb{Q}} \text{Fil}_{k-1,l-1}^{\text{W,L}}(\text{qMZ}), \end{aligned}$$

because we have

$$\begin{aligned} \text{gr}_{k,l}^{\text{W,L}}(\text{qMZ}) &\cong \text{Fil}_l^{\text{L}} \left(\text{Fil}_k^{\text{W}}(\text{qMZ}) / \text{Fil}_{k-1}^{\text{W}}(\text{qMZ}) \right) \\ &\quad / \text{Fil}_{l-1}^{\text{L}} \left(\text{Fil}_k^{\text{W}}(\text{qMZ}) / \text{Fil}_{k-1}^{\text{W}}(\text{qMZ}) \right). \end{aligned}$$

Now using Theorem 5.4 we get all the black marked entries in Table 3. For the conjectured entries in Table 3 we assumed that all the entries in Table 2 were exact, except for the diagonals for which we guessed the entries for weight bigger than 11.

ii) The number of independent relations we found give all the black marked entries in Table 4, since by i) we know that there aren't more. The conjectured entries in

Table 4 equal the difference of the number of generators $a(k, l)$ of in $\text{gr}_{k,l}^{\text{W,L}}(\text{qMZ})$ minus the corresponding dimension conjectured in i). \square

Proof. (of Theorem 1.6) The entries in Table 1 were calculated from the values for $d'(k, l)$ given in Theorem 5.5 by means of the formula given in Proposition 5.3. Actually we have double-checked this table with the computer. \square

Remark 5.6. Of course a lot of the conjectured relations in the table of Theorem 5.5 can be obtained by using the methods mentioned in this paper. We expect that with a more detailed study of the kind of relations we can obtain so far we could derive much better results and we plan to come back to this in future [Ba2].

Remark 5.7. The lower bounds where proven with the help of a computer and we expect that our program has found all the linear independent elements. We therefore conjecture that Table 3 in Theorem 5.5 gives the exact values of $d'(k, l)$ for all k, l we have tested. Assuming this we can ask for relations that are satisfied by the $d'(k, l)$. We observe that $d'_k = \sum_{l=1}^k d'(k, l)$ satisfies: $d'_0 = 1, d'_1 = 0, d'_2 = 1$ and

$$d'_k = 2d'_{k-2} + 2d'_{k-3}, \quad \text{for } 5 \leq k \leq 11.$$

We see no reason why this shouldn't hold for all $k > 11$ also, i.e. we ask whether

$$\sum_{k \geq 0} \text{gr}_k^{\text{W}}(\text{qMZ})x^k = \sum_{k \geq 0} d'_k x^k \stackrel{?}{=} \frac{1 - x^2 + x^4}{1 - 2x^2 - 2x^3}. \quad (5.4)$$

Even more speculative we may ask whether there a polynomial $P(x, y), Q(x, y) \in \mathbb{Q}[x, y]$ such that

$$\sum_{k,l \geq 0} \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\text{qMZ})x^k y^l = \sum_{k,l \geq 0} d'(k, l)x^k y^l \stackrel{?}{=} \frac{P(x, y)}{Q(x, y)}. \quad (5.5)$$

and $\frac{P(x,1)}{Q(x,1)} = \frac{1-x^2+x^4}{1-2x^2-2x^3}$. In fact, for the data we have so far there exist a family of polynomials $P(x, y)$ and $Q(x, y)$ such that if $\frac{P(x,y)}{Q(x,y)} = \sum a(k, l)x^k y^l$, then $d'(k, l) = a(k, l)$ for all $d'(k, l)$ in table in Theorem 3.

A general reason why such conjectural formulas may hold is that these are analogous to the Zagier conjecture for the dimension d_k of MZ_k

$$\sum_{k \geq 0} \dim_{\mathbb{Q}} \text{gr}_k^{\text{W}}(\text{MZ})X^k = \sum_{k \geq 0} d_k X^k \stackrel{?}{=} \frac{1}{1 - X^2 - X^3}$$

and its refinement by the Broadhurst Kreimer conjecture

$$\sum_{\substack{k \geq 0 \\ l \geq 0}} \dim_{\mathbb{Q}} \text{gr}_{k,l}^{\text{W,L}}(\mathcal{MZ}) X^k Y^l \stackrel{?}{=} \frac{1 + \mathbb{E}(X)Y}{1 - \mathbb{O}(X)Y + \mathbb{S}(X)Y^2 - \mathbb{S}(X)Y^4}.$$

where

$$\mathbb{E}(X) = \frac{X^2}{1 - X^2}, \quad \mathbb{O}(X) = \frac{X^3}{1 - X^2}, \quad \mathbb{S}(X) = \frac{X^{12}}{(1 - X^4)(1 - X^6)}.$$

We finally observe that conjecturally the algebra $q\mathcal{MZ}$ is much bigger than \mathcal{MZ} as we read of the following table.

k	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
d_k	1	0	1	1	1	2	2	3	4	5	7	9	12	16	21	28	37
d'_k	1	0	1	2	3	6	10	18	32	56	100	176	312	552	976	1728	3056

Table 5: First values of d_k and d'_k .

6 Interpretation as a q -analogue of multiple zeta values

We will show that the brackets can be seen as an q -analogue of multiple zeta values.

Remark 6.1. The most common example for an q -analogue of multiple zeta values are the multiple q -zeta values (see for example [Br]). They are defined for $s_1 > 1, s_2, \dots, s_l \geq 1$ as

$$\zeta_q(s_1, \dots, s_l) = \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{q^{n_j(s_j-1)}}{[n_j]_q^{s_j}}, \quad (6.1)$$

where one has to be careful with the notation here, because the brackets $[n]_q$ in this case denote the q -analogue of a natural number n_j . They are given by

$$[n]_q = \frac{1 - q^n}{1 - q} = \sum_{j=0}^{n-1} q^j.$$

With this it is easy to see that since $s_1 > 1$

$$\lim_{q \rightarrow 1} \zeta_q(s_1, \dots, s_l) = \zeta(s_1, \dots, s_l).$$

These function also fulfill a lot of relations from which one can deduce relations of MZV due to the limiting process.

It seems strange to us, that albeit the cases $(1 - q)^s[s]$ have been treated as q -zeta values [Zu], [Pu] or [KKW] the definition (6.1) has become standard (see e.g. [Br], [Zh],[OKZ]) and not $(1 - q)^{s_1+\dots+s_k}[s_1, \dots, s_l]$.

Remark 6.2. There is also another q -analogue, which is more directly connected to the brackets. It is defined by

$$\begin{aligned}\bar{\zeta}_q(s_1, \dots, s_l) &= (1 - q)^{-k} \zeta_q(s_1, \dots, s_l) \\ &= \sum_{n_1 > \dots > n_l > 0} \frac{q^{n_1(s_1-1)} \dots q^{n_l(s_l-1)}}{(1 - q^{n_1})^{s_1} \dots (1 - q^{n_l})^{s_l}}\end{aligned}$$

and which are called modified q -multiple zeta values in [OT] or [Ta].

If all $s_j > 1$, then modified q -multiple zeta values can be written in terms of brackets, which follows from the fact that the Eulerian polynomials form a basis of a certain space of polynomials [BK]. Clearly one has $\bar{\zeta}_q(2, \dots, 2) = [2, \dots, 2]$ because $P_1(t) = 1$. If all indices $s_j \geq 2$ the connection gets a little bit more complicated. For example it is

$$\bar{\zeta}_q(4) = [4] - [3] + \frac{1}{3}[2],$$

and this is due to the identity

$$\frac{t^3}{(1 - t)^4} = \frac{tP_3(t)}{3!(1 - t)^4} - \frac{tP_2(t)}{2!(1 - t)^3} + \frac{1}{3} \frac{tP_1(t)}{(1 - t)^2}.$$

When one of the s_j is equal to 1 we don't expect such a simple connection. But still there seems to be a connections if $s_1 > 1$, for example

$$\bar{\zeta}_q(2, 1) \equiv [2, 1] - [2] + d[1] \pmod{q^{100}\mathbb{Q}[[q]]}.$$

It is not difficult to check that the space of modified q -multiple zeta is closed under multiplication (see e.g. [HI], p. 2). However, the algebra of admissible brackets $q\mathcal{MZ}$ is not isomorphic to the \mathbb{Q} -algebra of modified q -multiple zeta values in the sense of [OT] or [Ta]. This is in essence due to the relation $\bar{\zeta}_q(2, 1) = \bar{\zeta}_q(3)$ in contrast to $[2, 1] \neq [3]$.

Definition 6.3. For $k \in \mathbb{N}$ we define the map $Z_k : \text{Fil}_k^{\text{W}}(q\mathcal{MZ}) \rightarrow \mathbb{R}$ by

$$Z_k([s_1, \dots, s_l]) = \lim_{q \rightarrow 1} ((1 - q)^k [s_1, \dots, s_l]).$$

Proposition 6.4. The map Z_k is linear and on the generators of $\text{Fil}_k^W(\mathfrak{qMZ})$, i.e., on brackets with $s_1 > 0$, it is given by

$$Z_k([s_1, \dots, s_l]) = \begin{cases} \zeta(s_1, \dots, s_l), & k = s_1 + \dots + s_l, \\ 0, & k > s_1 + \dots + s_l. \end{cases}$$

Proof. Using Lemma 2.5 and Lemma 6.6 below, we derive for $k = s_1 + \dots + s_l$

$$\begin{aligned} Z_k([s_1, \dots, s_l]) &= \lim_{q \rightarrow 1} ((1-q)^k [s_1, \dots, s_l]) \\ &= \lim_{q \rightarrow 1} \left((1-q)^k \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{q^{n_j} P_{s_j-1}(q^{n_j})}{(s_j-1)! (1-q^{n_j})^{s_j}} \right) \\ &= \sum_{n_1 > \dots > n_l > 0} \lim_{q \rightarrow 1} \prod_{j=1}^l \frac{(1-q)^{s_j} q^{n_j} P_{s_j-1}(q^{n_j})}{(1-q^{n_j})^{s_j} (s_j-1)!} \\ &= \zeta(s_1, \dots, s_l); \end{aligned}$$

here we used that the k -th Eulerian polynomial $P_k(t)$ satisfies $P_k(1) = k!$. If $k > s_1 + \dots + s_l$ it is $Z_k([s_1, \dots, s_l]) = \lim_{q \rightarrow 1} (1-q)^{k-s_1-\dots-s_l} \zeta(s_1, \dots, s_l) = 0$. In Lemma 6.6 we will justify the interchange of the limit and the summation. \square

Corollary 6.5. Let $f = \sum_{n \geq 0} a_n q^n$ be a quasi-modular form of weight k . Then the map Z_k sends f to $(-2\pi i)^k a_0$. The space S_k of weight k cusp-forms is therefore a subspace of the kernel of Z_k .

Proof. Any quasi-modular form of weight k can be written as a homogenous polynomial in G_2, G_4 and G_6 , therefore $\widetilde{M}_k(\Gamma_1) \subset \mathcal{Q}_k$. Since Z_k is a linear operator we can focus on the monomials. Let us consider the most simplest case first. For $a, b \in \{2, 4, 6\}$ we have

$$Z_{a+b}(G_a G_b) = \lim_{q \rightarrow 1} (1-q)^{a+b} G_a G_b = \lim_{q \rightarrow 1} (1-q)^a G_a \lim_{q \rightarrow 1} (1-q)^b G_b = Z_a(G_a) Z_b(G_b)$$

and by Proposition 6.4 we have $Z_a(G_a) Z_b(G_b) = \zeta(a) \zeta(b)$ which is exactly $(-2\pi i)^{a+b}$ times the constant term of $G_a G_b$. The same argument holds for more general monomials and therefore the claim follows. \square

Lemma 6.6. i) Define a series $\{F_M(q)\}_{M \in \mathbb{N}}$ by

$$F_M(q) = \sum_{M \geq n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{(1-q)^{s_j} q^{n_j} P_{s_j-1}(q^{n_j})}{(1-q^{n_j})^{s_j} (s_j-1)!},$$

then it converges uniformly to $(1-q)^k [s_1, \dots, s_l]$ for q in the interval $[0, 1]$ and therefore

$$\lim_{q \rightarrow 1} ((1-q)^k [s_1, \dots, s_l]) = \sum_{n_1 > \dots > n_l > 0} \lim_{q \rightarrow 1} \prod_{j=1}^l \frac{(1-q)^{s_j} q^{n_j} P_{s_j-1}(q^{n_j})}{(1-q^{n_j})^{s_j} (s_j-1)!} \quad (6.2)$$

ii) Let $k, n \in \mathbb{N}$ be natural numbers and define the function

$$f_{k,n}(q) = \frac{(1-q)^k q^n P_{k-1}(q^n)}{(1-q^n)^k (k-1)!},$$

then for $q \in [0, 1]$ it is $f_{1,n}(q) \leq \frac{1}{n}$ and for $k > 1$ we have $f_{k,n}(q) \leq \frac{1}{n^2}$.

Proof. We start with the proof of ii) because we need it for the proof of i). It is

$$f_{1,n}(q) = \frac{(1-q)q^n}{(1-q^n)}$$

because $P_0(q^n) = 1$. This is bounded by $\frac{1}{n}$ because the function

$$b_n(q) = n(1-q)q^n - (1-q^n)$$

is negative for all $q \in (0, 1)$ which can be seen by $b_n(1) = 0$ and the fact that the derivative

$$b'_n(q) = n^2(1-q)q^{n-1} + n(q^{n-1} - q^n).$$

is positive. We will show that

$$\frac{(1-q)^2 q^n}{(1-q^n)^2} \cdot \frac{P_{k-1}(q^n)}{(k-1)!} \leq \frac{1}{n^2}$$

for all k . This will be sufficient ii) for proving the statement for all $k \geq 2$ because it is $\frac{1-q}{1-q^n} < 1$ for $q \in (0, 1)$. Because of the positivity of the coefficients of $P_{k-1}(q)$ and $P_{k-1}(1) = (k-1)!$ we have for $q \in (0, 1)$ that

$$\frac{P_{k-1}(q^n)}{(k-1)!} \leq 1.$$

It therefore remains to show that

$$h_n(q) := \frac{(1-q)^2 q^n}{(1-q^n)^2} - \frac{1}{n^2} \stackrel{!}{\leq} 0.$$

We will do this by showing that $h_n(q)$ is monotonically increasing in the desired interval and

$$\lim_{q \rightarrow 1} h_n(q) = 0.$$

The latter can be seen by using l'hospital twice. For the monotonicity we first derive the derivative of h :

$$h'_n(q) = \frac{-(1-q)q^{n-1}}{(1-q^n)^3} \cdot (2q(1-q^n) - n(1-q)(1+q^n)).$$

The first factor is negative and we therefore just have to proof that the term in the brackets is also negative for all $n \in \mathbb{N}$ and $q \in (0, 1)$ which we will do by induction on n . For $n = 1$ this is trivial and for the inductive step we first rewrite the statement as

$$2 \frac{q(1-q^n)}{(1-q)} = 2 \sum_{j=1}^n q^j \leq n(1+q^n).$$

Assuming that this holds for an n we can write

$$2 \sum_{j=1}^{n+1} q^j = 2 \sum_{j=1}^n q^j + 2q^{n+1} \leq n(1+q^n) + 2q^{n+1}.$$

Now we have to show that

$$n(1+q^n) + 2q^{n+1} \stackrel{!}{\leq} (n+1)(1+q^{n+1})$$

which we again do by first setting

$$g_n(q) := (n+1)(1+q^{n+1}) - (n(1+q^n) + 2q^{n+1}) = n(q^{n-1} - q^n) + 1 - q^{n+1}$$

and then noticing that $g_n(1) = 0$. The derivative $g'_n(q) = -q^{n-1}(n^2(1-q) + q)$ is clearly negative for $q \in (0, 1)$ which implies $g_n(q) \geq 0$ and therefore finishes the inductive step.

We now prove i). Using the bounds in ii) and taking into account $s_1 > 1$ we have the bound

$$\begin{aligned} F_M(q) &= \sum_{M \geq n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{(1-q)^{s_j} q^{n_j} P_{s_j-1}(q^{n_j})}{(1-q^{n_j})^{s_j} (s_j-1)!} \\ &\leq \sum_{M \geq n_1 > \dots > n_l > 0} \frac{1}{n_1^2 n_2 \dots n_l} \leq \zeta(2, 1, \dots, 1) \end{aligned}$$

for $q \in [0, 1]$ and all $M > 0$. Therefore the sum on the right-hand side of (6.2) converges uniformly as a function in q and therefore we can interchange limit and summation. \square

Remark 6.7. In [Pu] it is shown $[1] \approx -\frac{\log(1-q)}{1-q}$ near $q = 1$. Since a bracket $[s_1, \dots, s_l]$ with $s_1 = 1$ are polynomials in $[1]$, it is clear that Z_k can't be extended as an analytical map as given in Definition 6.3 to all $\text{Fil}_k^W(\mathcal{MD})$.

7 Applications to multiple zeta values

As mentioned in the introduction we now want to consider a direct connection of brackets with multiple zeta values (MZV).

We start by defining for any $\rho \in \mathbb{R}_{\geq 1}$ the following spaces

$$\mathcal{Q}_\rho = \left\{ \sum_{n>0} a_n q^n \in \mathbb{R}[[q]] \mid a_n = O(n^{\rho-1}) \right\}$$

and

$$\mathcal{Q}_{<\rho} = \left\{ \sum_{n>0} a_n q^n \in \mathbb{R}[[q]] \mid \exists \varepsilon > 0 \text{ with } a_n = O(n^{\rho-1-\varepsilon}) \right\},$$

where $a_n = O(n^{\rho-1})$ is the usual big O notation which means that there is an $C \in \mathbb{R}$ with $|a_n| \leq Cn^{\rho-1}$ for all $n \in \mathbb{N}$.

Lemma 7.1. i) Both $\mathcal{Q}_{<\rho}$ and \mathcal{Q}_ρ are \mathbb{R} vector spaces.

ii) We have $\mathcal{Q}_{\rho-1} \subset \mathcal{Q}_{<\rho} \subset \mathcal{Q}_\rho$.

iii) Let $r, s \in \mathbb{R}_{\geq 1}$ then

$$\mathcal{Q}_{<r} \cdot \mathcal{Q}_{<s} \subset \mathcal{Q}_{<r+s}, \quad \mathcal{Q}_{<r} \cdot \mathcal{Q}_s \subset \mathcal{Q}_{<r+s} \quad \text{and} \quad \mathcal{Q}_r \cdot \mathcal{Q}_s \subset \mathcal{Q}_{r+s}.$$

Proof. It is obvious that i) and ii) hold. For iii) we consider $f = \sum_{n>0} a_n q^n \in \mathcal{Q}_r$, $g = \sum_{n>0} b_n q^n \in \mathcal{Q}_s$. Then by definition $|a_n| \leq C_1 n^{r-1}$ and $|b_n| \leq C_2 n^{s-1}$ for some constants C_1 and C_2 . Setting $f \cdot g = \sum_{n>0} c_n q^n$ we derive

$$|c_n| = \left| \sum_{n_1+n_2=n} a_{n_1} b_{n_2} \right| \leq C_1 C_2 \sum_{n_1+n_2=n} n_1^{r-1} n_2^{s-1} \leq C_1 C_2 n \cdot n^{r-1} n^{s-1} = O(n^{r+s-1}).$$

and therefore $f \cdot g \in \mathcal{Q}_{r+s}$. By similar considerations the remaining cases follow. \square

Proposition 7.2. For $\rho > 1$ define the map Z_ρ for a $f = \sum_{n>0} a_n q^n \in \mathbb{R}[[q]]$ by

$$Z_\rho(f) = \limsup_{q \rightarrow 1} (1-q)^\rho \sum_{n>0} a_n q^n,$$

where one assumes $q \in (0, 1)$. Then the following statements are true

i) Z_ρ is a linear map from \mathcal{Q}_ρ to \mathbb{R}

ii) $\mathcal{Q}_{<\rho} \subset \ker Z_\rho$.

iii) $\mathcal{Q}_{<\rho-1} \subset \ker(Z_\rho)$, where as before $d = q \frac{d}{dq}$.

Proof. We prove i) and ii) simultaneously. In order to do this we use the following expression for the polylogarithm

$$\text{Li}_{-s}(q) = \Gamma(1+s)(-\log q)^{-s-1} + \sum_{n=0}^{\infty} \frac{\zeta(-s-n)}{n!} (\log q)^n$$

which is valid for $s \neq -1, -2, -3, \dots$, $|z| < 1$ and where $\zeta(-s-n)$ is the analytic continuation of the Riemann zeta-function. The proof of this can be found in [CG] Corollary 2.1. The logarithm has the following expansion near $q = 1$

$$-\log(q) = \sum_{n=1}^{\infty} \frac{(1-q)^n}{n}.$$

Using this one gets for $\varepsilon \geq 0$

$$\begin{aligned} \limsup_{q \rightarrow 1} (1-q)^\rho \sum_{n>0} n^{\rho-1-\varepsilon} q^n &= \lim_{q \rightarrow 1} (1-q)^\rho \text{Li}_{\varepsilon+1-\rho}(q) \\ &= \limsup_{q \rightarrow 1} (1-q)^\rho \left(\Gamma(\rho-\varepsilon)(-\log q)^{-\rho+\varepsilon} + \sum_{n=0}^{\infty} \frac{\zeta(-\rho+\varepsilon-n)}{n!} (\log q)^n \right) \\ &= \Gamma(\rho-\varepsilon) \limsup_{q \rightarrow 1} \frac{(1-q)^\rho}{\left(\sum_{n=1}^{\infty} \frac{(1-q)^n}{n} \right)^{\rho-\varepsilon}} = \begin{cases} \Gamma(\rho), & \varepsilon = 0 \\ 0, & \varepsilon > 0 \end{cases}. \end{aligned}$$

Now assume that for a $\varepsilon \geq 0$ we have $f = \sum_{n>0} a_n q^n$ with $|a_n| \leq C \cdot n^{\rho-1-\varepsilon}$, i.e. $f \in \mathcal{Q}_\rho$ for $\varepsilon = 0$ and $f \in \mathcal{Q}_{<\rho}$ for $\varepsilon > 0$, then the calculation above gives

$$|Z_\rho(f)| = \left| Z_\rho \left(\sum_{n>0} a_n q^n \right) \right| \leq C \cdot Z_\rho \left(\sum_{n>0} n^{\rho-1-\varepsilon} \right) = \begin{cases} C \cdot \Gamma(\rho), & \varepsilon = 0 \\ 0, & \varepsilon > 0 \end{cases}$$

and therefore $Z_\rho(f) \in \mathbb{R}$ and $Z_\rho(f) = 0$ respectively.

For iii) we just have to observe that the derivative $d = q \frac{d}{dq}$ on $\sum_{n>0} a_n q^n$ is given by $\sum_{n>0} n a_n q^n$. With this it is clear that with i) we obtain $d(\mathcal{Q}_{<\rho-1}) \subset \mathcal{Q}_{<\rho} \subset \ker(Z_\rho)$. \square

The brackets $[s_1, \dots, s_l]$ can be considered as elements in the spaces we studied above.

Proposition 7.3. i) For any s_1, \dots, s_l we have $[s_1, \dots, s_l] \in \mathcal{Q}_{<s_1+\dots+s_l+1}$.

ii) If all $s_1, s_2, \dots, s_l > 1$, then $[s_1, \dots, s_l] \in \mathcal{Q}_{s_1+\dots+s_l}$.

iii) For any s_1, \dots, s_l we have

$$[s_1, \dots, s_l] \subset \ker(Z_{s_1+\dots+s_l+1})$$

and

$$d[s_1, \dots, s_l] \subset \ker(Z_{s_1+\dots+s_l+2})$$

Proof. We begin with the proof of ii). It is a well-known fact that for $s > 1$ the divisor sums $\sigma_{s-1}(n)$ are in $O(n^{s-1})$ and therefore $[s] \in \mathcal{Q}_s$. Then by Lemma 7.1 iii) we have $\sum_{n>0} a_{s_1, \dots, s_l}(n)q^n := [s_1] \dots [s_l] \in \mathcal{Q}_{s_1+\dots+s_l}$. It is clearly

$$\begin{aligned} \sigma_{s_1-1, \dots, s_l-1}(n) &= \sum_{\substack{u_1 v_1 + \dots + u_l v_l = n \\ u_1 > \dots > u_l > 0}} v_1^{s_1-1} \dots v_l^{s_l-1} \\ &\leq \sum_{u_1 v_1 + \dots + u_l v_l = n} v_1^{s_1-1} \dots v_l^{s_l-1} = a_{s_1, \dots, s_l}(n), \end{aligned}$$

which implies $[s_1, \dots, s_l] \in \mathcal{Q}_{s_1+\dots+s_l}$.

In order to show i) we can use the same argument as in ii) except that one has $\sigma_0(n) \in O(\log(n)) \subset O(n^\varepsilon)$ for any $\varepsilon > 0$. Using this we obtain $[1] \in \mathcal{Q}_{<2}$ and therefore $[s_1, \dots, s_l] \in \mathcal{Q}_{<s_1+\dots+s_l+1}$ for $s_1, \dots, s_l \geq 1$.

Finally iii) is an immediate consequence of Proposition 7.2 ii) and iii). \square

Using $\mathcal{MD} = \mathfrak{q}\mathcal{MZ}[[1]]$ we define a map

$$\begin{aligned} Z_k^{alg} : \text{Fil}_k^{\text{W}}(\mathcal{MD}) &\longrightarrow \mathbb{R}[T], \\ Z_k^{alg} \left(\sum_{j=0}^k g_j [1]^{k-j} \right) &= \sum_{j=0}^k Z_j(g_j) T^{k-j} \in \mathbb{R}[T], \end{aligned}$$

where $g_j \in \text{Fil}_j^{\text{W}}(\mathfrak{q}\mathcal{MZ})$.

Proposition 7.4. For all $f \in \text{Fil}_k^{\text{W}}(\mathcal{MD})$ it is $Z_{k+2}^{alg}(df) = 0$.

Proof. An element in $\text{Fil}_k^{\text{W}}(\mathcal{MD})$ can be written as $\sum_{j=0}^k g_j [1]^{k-j}$ with $g_j \in \text{Fil}_j^{\text{W}}(\mathfrak{q}\mathcal{MZ})$. The map Z_k^{alg} is linear, it therefore suffices to prove the statement for a $f \in \text{Fil}_k^{\text{W}}(\mathcal{MD})$ of the form $f = g_j [1]^{k-j}$. The derivative of this f is given by

$$df = dg_j \cdot [1]^{k-j} + (k-j)g_j d[1] \cdot [1]^{k-j-1}.$$

As we saw before it is $d[1] = [3] + \frac{1}{2}[2] - [2, 1] \in \mathfrak{q}\mathcal{MZ}$ and by Proposition 3.14 it is $dg_j \in \mathfrak{q}\mathcal{MZ}$. The map Z_{k+2}^{alg} is therefore given on df by

$$Z_{k+2}^{alg}(df) = Z_{j+2}(dg_j) T^{k-j} + (k+j)Z_{j+3}(g_j d[1]) T^{k-j-1}.$$

It is $Z_{j+3}(g_j d[1]) = Z_j(g_j) \cdot Z_3(d[1])$ and by Proposition 7.3 we obtain $Z_3(d[1]) = Z_{j+2}(dg_j) = 0$ from which the statement follows \square

Remark 7.5. The authors also expect that the implication

$$Z_k(f) = 0 \implies Z_k^{alg}(f) = 0$$

holds for arbitrary $f \in \mathcal{MD}$.

Now Theorem 1.13 follows by Proposition 7.3 and Proposition 7.4. Using these propositions we are able to derive relations between MZV coming from elements in the kernel of the map Z_k . We give a few examples which give a new interpretation of well known identities of multiple zeta values.

Example 7.6. i) We have seen earlier that the derivative of [1] is given by

$$d[1] = [3] + \frac{1}{2}[2] - [2, 1]$$

and because of the proposition it is $d[1], [2] \in \ker Z_3$ from which $\zeta(2, 1) = \zeta(3)$ follows.

ii) (Shuffle product) Proposition 3.3 stated for $s_1 + s_2 = k + 2$ that

$$\binom{k}{s_1 - 1} \frac{d[k]}{k} = [s_1] \cdot [s_2] + \binom{k}{s_1 - 1} [k+1] - \sum_{a+b=k+2} \left(\binom{a-1}{s_1-1} + \binom{a-1}{s_2-1} \right) [a, b].$$

Applying Z_{k+2} on both sides we obtain the shuffle product for single zeta values

$$\zeta(s_1) \cdot \zeta(s_2) = \sum_{a+b=k+2} \left(\binom{a-1}{s_1-1} + \binom{a-1}{s_2-1} \right) \zeta(a, b).$$

Example 7.7. For the cusp form $\Delta \in S_{12} \subset \ker(Z_{12})$ we derived the representation

$$\begin{aligned} \frac{1}{2^6 \cdot 5 \cdot 691} \Delta &= 168[5, 7] + 150[7, 5] + 28[9, 3] \\ &+ \frac{1}{1408}[2] - \frac{83}{14400}[4] + \frac{187}{6048}[6] - \frac{7}{120}[8] - \frac{5197}{691}[12]. \end{aligned}$$

Letting Z_{12} act on both sides one obtains the relation

$$\frac{5197}{691} \zeta(12) = 168\zeta(5, 7) + 150\zeta(7, 5) + 28\zeta(9, 3).$$

In general it is known due to [GKZ] that every cusp form of weight k give rise to a relation between double zeta values with odd entries modulo $\zeta(k)$. We believe that one can give an alternative proof of his fact with the help of brackets.

At the end we want to mention a curious property of the brackets which seems to appear at length 3. Fixing a weight k and a length l one could ask, if there are linear relations between brackets $[s_1, \dots, s_l]$ with the same weight $s_1 + \dots + s_l = k$ and length l . For $l = 2$ using the computer the authors could not find any such relations up to weight 30. But for $l = 3$ there seem to be relations of this form starting in weight 9. The first two of them are given by:

Conjecture 7.8. In $\text{Fil}_{9,3}^{\text{W,L}}(\mathcal{MD})$ and $\text{Fil}_{10,3}^{\text{W,L}}(\mathcal{MD})$ we have the relation

$$\begin{aligned} 0 = & \frac{9}{5} [2, 3, 4] + 2 [2, 4, 3] - [2, 5, 2] \\ & + 2 ([3, 5, 1] - [3, 1, 5]) - \frac{1}{5} [3, 2, 4] - [3, 3, 3] - [3, 4, 2] \\ & + \frac{3}{5} ([4, 4, 1] - [4, 1, 4]) - \frac{11}{10} [4, 2, 3] + \frac{1}{2} [4, 3, 2] \\ & + \frac{4}{5} ([5, 1, 3] - [5, 3, 1]) - [6, 1, 2] + [6, 2, 1]. \end{aligned}$$

and

$$\begin{aligned} 0 = & \frac{4}{3} [2, 3, 5] + \frac{14}{5} [2, 4, 4] + \frac{29}{15} [2, 5, 3] - [2, 6, 2] \\ & + 2 ([3, 6, 1] - [3, 1, 6]) - \frac{2}{3} [3, 2, 5] + \frac{2}{5} [3, 3, 4] - \frac{1}{15} [3, 4, 3] - [3, 5, 2] \\ & + 2 ([4, 5, 1] - [4, 1, 5]) - \frac{6}{5} [4, 2, 4] - \frac{4}{3} [4, 3, 3] - \frac{2}{5} [4, 4, 2] \\ & + \frac{2}{5} ([5, 4, 1] - [5, 1, 4]) - [5, 2, 3] + \frac{1}{5} [5, 3, 2] \\ & + \frac{1}{3} ([6, 1, 3] - [6, 3, 1]) - [7, 1, 2] + [7, 2, 1]. \end{aligned}$$

Notice that these are all elements in $\text{Fil}_9^{\text{W}}(\text{qMZ})$ (resp. $\text{Fil}_{10}^{\text{W}}(\text{qMZ})$) and therefore a relation for triple zeta values would follow from this. There are similar relations in higher weights and computations show the following:

k	1-8	9	10	11	12	13	14	15	16	17	18	19	20
t_k	0	1	1	3	6	8	12	16	21	25	32	37	45

Table 6: Conjectured numbers t_k of relations between $[a, b, c]$ with $a + b + c = k$.

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E-mail:

henrik.bachmann@math.uni-hamburg.de
kuehn@math.uni-hamburg.de

FACHBEREICH MATHEMATIK (AZ)
UNIVERSITÄT HAMBURG
BUNDESSTRASSE 55
D-20146 HAMBURG

Appendix B

The double shuffle relations for multiple Eisenstein series

The double shuffle relations for multiple Eisenstein series

Henrik Bachmann*, Koji Tasaka†

Abstract

We study the multiple Eisenstein series introduced by Gangl, Kaneko and Zagier. We give a proof of (restricted) finite double shuffle relations for multiple Eisenstein series by revealing an explicit connection between the Fourier expansion of multiple Eisenstein series and the Goncharov coproduct on Hopf algebras of iterated integrals.

Keywords: Multiple zeta value, Multiple Eisenstein series, The Goncharov coproduct, Modular forms, Double shuffle relation.

Subclass[2010]: 11M32, 11F11, 13J05, 33E20.

1 Introduction

The purpose of this paper is to study the multiple Eisenstein series, which are holomorphic functions on the upper half-plane $\{\tau \in \mathbb{C} \mid \text{Im}(\tau) > 0\}$ and which can be viewed as a multivariate generalisation of the classical Eisenstein series, defined as an iterated multiple sum

$$G_{n_1, \dots, n_r}(\tau) = \sum_{\substack{0 < \lambda_1 < \dots < \lambda_r \\ \lambda_1, \dots, \lambda_r \in \mathbb{Z}\tau + \mathbb{Z}}} \frac{1}{\lambda_1^{n_1} \dots \lambda_r^{n_r}} \quad (n_1, \dots, n_{r-1} \in \mathbb{Z}_{\geq 2}, n_r \in \mathbb{Z}_{\geq 3}), \quad (1.1)$$

*email : henrik.bachmann@uni-hamburg.de, Universität Hamburg

†email : koji.tasaka@math.nagoya-u.ac.jp, Graduate School of Mathematics, Nagoya University

where the positivity $l\tau + m \succ 0$ of a lattice point is defined to be either $l > 0$ or $l = 0, m > 0$, and $l\tau + m \succ l'\tau + m'$ means $(l - l')\tau + (m - m') \succ 0$. These functions were first introduced and studied by Gangl, Kaneko and Zagier [7, Section 7], where they investigated the double shuffle relation satisfied by double zeta values for the double Eisenstein series $G_{n_1, n_2}(\tau)$. Here the double zeta value is the special case of multiple zeta values defined by

$$\zeta(n_1, \dots, n_r) = \sum_{\substack{0 < m_1 < \dots < m_r \\ m_1, \dots, m_r \in \mathbb{Z}}} \frac{1}{m_1^{n_1} \dots m_r^{n_r}} \quad (n_1, \dots, n_{r-1} \in \mathbb{Z}_{\geq 1}, n_r \in \mathbb{Z}_{\geq 2}). \quad (1.2)$$

Their results were extended to the double Eisenstein series for higher level (congruence subgroup of level N) in [12] ($N = 2$) and in [16] (N : general), and have interesting applications to the theory of modular forms (see [15]) as well as the study of double zeta values of level N . Our aim of this paper is to give a framework of and a proof of double shuffle relations for multiple Eisenstein series.

The double shuffle relation, or rather, the finite double shuffle relation (cf. e.g. [10]) describes a collection of \mathbb{Q} -linear relations among multiple zeta values arising from two ways of expressing multiple zeta values as iterated sums (1.2) and as iterated integrals (3.1). Each expression produces an algebraic structure on the \mathbb{Q} -vector space spanned by all multiple zeta values. The product associated to (1.2) (resp. (3.1)) is called the harmonic product (resp. shuffle product). For example, using the harmonic product, we have

$$\zeta(3)\zeta(3) = 2\zeta(3, 3) + \zeta(6),$$

and by the shuffle product formulas one obtains

$$\zeta(3)\zeta(3) = 12\zeta(1, 5) + 6\zeta(2, 4) + 2\zeta(3, 3). \quad (1.3)$$

Combining these equations gives the relation

$$12\zeta(1, 5) + 6\zeta(2, 4) - \zeta(6) = 0.$$

For the multiple Eisenstein series (1.1), it is easily seen that the har-

monic product formulas hold when the series defining $G_{n_1, \dots, n_r}(\tau)$ converges absolutely, i.e. $n_1, \dots, n_{r-1} \in \mathbb{Z}_{\geq 2}$ and $n_r \in \mathbb{Z}_{\geq 3}$, but the shuffle product is not the case – the shuffle product formula (1.3) replacing ζ with G does not make sense because an undefined multiple Eisenstein series $G_{1,5}(\tau)$ is involved. This paper develops the shuffle product of multiple Eisenstein series by revealing an explicit connection between the multiple Eisenstein series and the Goncharov coproduct, and as a consequence the validity of a restricted version of the finite double shuffle relations for multiple Eisenstein series is obtained.

This paper begins by computing the Fourier expansion of $G_{n_1, \dots, n_r}(\tau)$ for $n_1, \dots, n_r \geq 2$ (the case $n_r = 2$ will be treated by a certain limit argument in Definition 2.1) in Section 2. The Fourier expansion is deeply related with the Goncharov coproduct Δ (see (3.4)) on Hopf algebras of iterated integrals introduced by Goncharov [8, Section 2], which was first observed by Kaneko in several cases and studied by Belcher [6]. His Hopf algebra $\mathcal{I}_\bullet(S)$ is reviewed in Section 3.2, and we will observe a relationship between the Fourier expansion and the Goncharov coproduct Δ in the quotient Hopf algebra $\mathcal{I}_\bullet^1 := \mathcal{I}_\bullet / \mathbb{I}(0; 0; 1)\mathcal{I}_\bullet$ ($\mathcal{I}_\bullet := \mathcal{I}_\bullet(\{0, 1\})$), which can not be seen in \mathcal{I}_\bullet . The space \mathcal{I}_\bullet^1 has a linear basis (Proposition 3.5)

$$\{I(n_1, \dots, n_r) \mid r \geq 0, n_1, \dots, n_r \in \mathbb{Z}_{>0}\},$$

and we will express the Goncharov coproduct $\Delta(I(n_1, \dots, n_r))$ as a certain algebraic combination of the above basis (Propositions 3.7 and 3.9). As an example of this expression, one can compute

$$\Delta(I(2, 3)) = I(2, 3) \otimes 1 + 3I(3) \otimes I(2) + 2I(2) \otimes I(3) + 1 \otimes I(2, 3).$$

The relationship is then obtained by comparing the formula for $\Delta(I(n_1, \dots, n_r))$ with the Fourier expansion of $G_{n_1, \dots, n_r}(\tau)$, which in the case of $r = 2$ can be found by (2.8) and (3.11). More precisely, let us define the \mathbb{Q} -linear maps $\mathfrak{z}^\mathfrak{m} : \mathcal{I}_\bullet^1 \rightarrow \mathbb{R}$ and $\mathfrak{g} : \mathcal{I}_\bullet^1 \rightarrow \mathbb{C}[[q]]$ given by $I(n_1, \dots, n_r) \mapsto \zeta^\mathfrak{m}(n_1, \dots, n_r)$ and $I(n_1, \dots, n_r) \mapsto g_{n_1, \dots, n_r}(q)$, where $\zeta^\mathfrak{m}(n_1, \dots, n_r)$ is the regularised multiple zeta value with respect to the shuffle product (see Definition 3.1) and $g_{n_1, \dots, n_r}(q)$ is the generating series of the multiple divisor sum appearing in

the Fourier expansion of multiple Eisenstein series (see (2.4)). For instance, by (2.8) we have

$$G_{2,3}(\tau) = \zeta(2, 3) + 3\zeta(3)g_2(q) + 2\zeta(2)g_3(q) + g_{2,3}(q),$$

and hence $(\mathfrak{z}^{\text{III}} \otimes \mathfrak{g}) \circ \Delta(I(2, 3)) = G_{2,3}(\tau)$. In general, we have the following theorem which is the first main result of this paper.

Theorem 1.1. *For integers $n_1, \dots, n_r \geq 2$ we have*

$$(\mathfrak{z}^{\text{III}} \otimes \mathfrak{g}) \circ \Delta(I(n_1, \dots, n_r)) = G_{n_1, \dots, n_r}(\tau) \quad (q = e^{2\pi\sqrt{-1}\tau}).$$

The maps $\Delta : \mathcal{I}_{\bullet}^1 \rightarrow \mathcal{I}_{\bullet}^1 \otimes \mathcal{I}_{\bullet}^1$ and $\mathfrak{z}^{\text{III}} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{R}$ are algebra homomorphisms (Propositions 3.4 and 3.6) but the map $\mathfrak{g} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{C}[[q]]$ is not an algebra homomorphism (see (4.1)). Thus we can not expect a validity of the shuffle product formulas for the q -series $(\mathfrak{z}^{\text{III}} \otimes \mathfrak{g}) \circ \Delta(I(n_1, \dots, n_r))$ ($n_1, \dots, n_r \in \mathbb{Z}_{\geq 1}$) which can be naturally regarded as an extension of $G_{n_1, \dots, n_r}(\tau)$ to the indices with $n_i = 1$.

We shall construct in Section 4.1 an algebra homomorphism $\mathfrak{g}^{\text{III}} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{C}[[q]]$ (Definition 4.3) using certain q -series, and in Section 4.2 we define a regularised multiple Eisenstein series (see Definition 4.5)

$$G_{n_1, \dots, n_r}^{\text{III}}(q) := (\mathfrak{z}^{\text{III}} \otimes \mathfrak{g}^{\text{III}}) \circ \Delta(I(n_1, \dots, n_r)) \in \mathbb{C}[[q]] \quad (n_1, \dots, n_r \in \mathbb{Z}_{\geq 1}).$$

It follows from the definition that the q -series $G_{n_1, \dots, n_r}^{\text{III}}(q)$ ($n_1, \dots, n_r \in \mathbb{Z}_{\geq 1}$) satisfy the shuffle product formulas. We will prove that $G_{n_1, \dots, n_r}^{\text{III}}(q)$ coincides with the Fourier expansion of $G_{n_1, \dots, n_r}(\tau)$ when $n_1, \dots, n_r \geq 2$ and $q = e^{2\pi\sqrt{-1}\tau}$ (Theorem 4.6). Then, combining the shuffle product of G^{III} 's and the harmonic product of G 's yields the double shuffle relation for multiple Eisenstein series, which is the second main result of this paper (see Theorem 4.7 for the detail).

Theorem 1.2. *The (restricted) finite double shuffle relations hold for $G_{n_1, \dots, n_r}^{\text{III}}(q)$ ($n_1, \dots, n_r \in \mathbb{Z}_{\geq 1}$).*

The organisation of this paper is as follows. In section 2, the Fourier expansion of the multiple Eisenstein series $G_{n_1, \dots, n_r}(\tau)$ is considered. In section

3, we first recall the regularised multiple zeta value and Hopf algebras of iterated integrals introduced by Goncharov. Then we define the map \mathfrak{z}^{m} that assigns regularised multiple zeta value to formal iterated integrals. We also present the formula expressing $\Delta(I(n_1, \dots, n_r))$ as a certain algebraic combination of $I(k_1, \dots, k_i)$'s, and finally proves Theorem 1.1. Section 4 gives the definition of the algebra homomorphism \mathfrak{g}^{m} and proves double shuffle relations for multiple Eisenstein series. A future problem with the dimension of the space of G^{m} 's will be discussed in the end of this section.

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2 The Fourier expansion of multiple Eisenstein series

2.1 Multiple Eisenstein series

In this subsection, we define the multiple Eisenstein series and consider its Fourier expansion.

Recall the computation of the Fourier expansion of $G_{n_1}(\tau)$, which is well-known (see also [7, Section 7]):

$$G_{n_1}(\tau) = \sum_{0 < l\tau + m} \frac{1}{(l\tau + m)^{n_1}} = \sum_{m > 0} \frac{1}{m^{n_1}} + \sum_{l > 0} \sum_{m \in \mathbb{Z}} \frac{1}{(l\tau + m)^{n_1}}$$

$$= \zeta(n_1) + \frac{(-2\pi\sqrt{-1})^{n_1}}{(n_1-1)!} \sum_{n>0} \sigma_{n_1-1}(n) q^n,$$

where $\sigma_k(n) = \sum_{d|n} d^k$ is the divisor function and $q = e^{2\pi\sqrt{-1}\tau}$. Here for the last equality we have used the Lipschitz formula

$$\sum_{m \in \mathbb{Z}} \frac{1}{(\tau+m)^{n_1}} = \frac{(-2\pi\sqrt{-1})^{n_1}}{(n_1-1)!} \sum_{0 < v_1} v_1^{n_1-1} q^{v_1} \quad (n_1 \geq 2). \quad (2.1)$$

When $n_1 = 2$, the above computation (the second equality) can be justified by using a limit argument which in general is treated in Definition 2.1 below. We remark that the function $G_{n_1}(\tau)$ is a modular form of weight n_1 for $\mathrm{SL}_2(\mathbb{Z})$ when n_1 is even (> 2) ($G_2(\tau)$ is called the quasimodular form) and a non-trivial holomorphic function even if n_1 is odd.

The following definition enables us to compute the Fourier expansion of $G_{n_1, \dots, n_r}(\tau)$ for integers $n_1, \dots, n_r \geq 2$ and coincides with the iterated multiple sum (1.1) when the series defining (1.1) converges absolutely, i.e. $n_1, \dots, n_{r-1} \geq 2$ and $n_r \geq 3$.

Definition 2.1. For integers $n_1, \dots, n_r \geq 2$, we define the holomorphic function $G_{n_1, \dots, n_r}(\tau)$ on the upper half-plane called the multiple Eisenstein series by

$$\begin{aligned} G_{n_1, \dots, n_r}(\tau) &:= \lim_{L \rightarrow \infty} \lim_{M \rightarrow \infty} \sum_{\substack{0 < \lambda_1 < \dots < \lambda_r \\ \lambda_i \in \mathbb{Z}_L \tau + \mathbb{Z}_M}} \frac{1}{\lambda_1^{n_1} \dots \lambda_r^{n_r}} \\ &= \lim_{L \rightarrow \infty} \lim_{M \rightarrow \infty} \sum_{\substack{0 < (l_1 \tau + m_1) < \dots < (l_r \tau + m_r) \\ -L \leq l_1, \dots, l_r \leq L \\ -M \leq m_1, \dots, m_r \leq M}} \frac{1}{(l_1 \tau + m_1)^{n_1} \dots (l_r \tau + m_r)^{n_r}}, \end{aligned}$$

where we set $\mathbb{Z}_M = \{-M, -M+1, \dots, -1, 0, 1, \dots, M-1, M\}$ for an integer $M > 0$.

The Fourier expansion of $G_{n_1, \dots, n_r}(\tau)$ for integers $n_1, \dots, n_r \geq 2$ is obtained by splitting up the sum into 2^r terms, which was first done in [7] for the case $r = 2$ and in [1] for the general case (they use the opposite convention, so that the λ_i 's are ordered by $\lambda_1 \succ \dots \succ \lambda_r \succ 0$). To describe

each term we introduce the holomorphic function $G_{n_1, \dots, n_r}(w_1 \cdots w_r; \tau)$ on the upper half-plane below. For convenience, we express the set P of positive elements in the lattice $\mathbb{Z}\tau + \mathbb{Z}$ as the disjoint union of two sets

$$\begin{aligned} P_{\mathbf{x}} &:= \{l\tau + m \in \mathbb{Z}\tau + \mathbb{Z} \mid l = 0 \wedge m > 0\}, \\ P_{\mathbf{y}} &:= \{l\tau + m \in \mathbb{Z}\tau + \mathbb{Z} \mid l > 0\}, \end{aligned}$$

i.e. $P_{\mathbf{x}}$ are the lattice points on the positive real axis, $P_{\mathbf{y}}$ are the lattice points in the upper half-plane and $P = P_{\mathbf{x}} \cup P_{\mathbf{y}}$. We notice that $\lambda_1 \prec \lambda_2$ is equivalent to $\lambda_2 - \lambda_1 \in P$. Let us denote by $\{\mathbf{x}, \mathbf{y}\}^*$ the set of all words consisting of letters \mathbf{x} and \mathbf{y} . For integers $n_1, \dots, n_r \geq 2$ and a word $w_1 \cdots w_r \in \{\mathbf{x}, \mathbf{y}\}^*$ ($w_i \in \{\mathbf{x}, \mathbf{y}\}$) we define

$$\begin{aligned} G_{n_1, \dots, n_r}(w_1 \cdots w_r) &= G_{n_1, \dots, n_r}(w_1 \cdots w_r; \tau) \\ &:= \lim_{L \rightarrow \infty} \lim_{M \rightarrow \infty} \sum_{\substack{\lambda_1 - \lambda_0 \in P_{w_1} \\ \vdots \\ \lambda_r - \lambda_{r-1} \in P_{w_r} \\ \lambda_1, \dots, \lambda_r \in \mathbb{Z}_L \tau + \mathbb{Z}_M}} \frac{1}{\lambda_1^{n_1} \cdots \lambda_r^{n_r}}, \end{aligned}$$

where $\lambda_0 := 0$. Note that in the above sum, adjoining elements $\lambda_i - \lambda_{i-1} = (l_i - l_{i-1})\tau + (m_i - m_{i-1}), \dots, \lambda_j - \lambda_{j-1} = (l_j - l_{j-1})\tau + (m_j - m_{j-1})$ are in $P_{\mathbf{x}}$ (i.e. $w_i = \cdots = w_j = \mathbf{x}$ with $i \leq j$) if and only if they satisfy $m_{i-1} < m_i < \cdots < m_j$ with $l_{i-1} = l_i = \cdots = l_j$ (since $(l-l')\tau + (m-m') \in P_{\mathbf{x}}$ if and only if $l = l'$ and $m < m'$), and hence the function $G_{n_1, \dots, n_r}(w_1 \cdots w_r)$ is expressible in terms of the following function:

$$\Psi_{n_1, \dots, n_r}(\tau) = \sum_{-\infty < m_1 < \cdots < m_r < \infty} \frac{1}{(\tau + m_1)^{n_1} \cdots (\tau + m_r)^{n_r}},$$

which was studied thoroughly in [3]. In fact, as is easily seen that the series defining $\Psi_{n_1, \dots, n_r}(\tau)$ converges absolutely when $n_1, \dots, n_r \geq 2$, we obtain the

following expression:

$$\begin{aligned} & G_{n_1, \dots, n_r}(w_1 \cdots w_r) \\ &= \zeta(n_1, \dots, n_{t_1-1}) \sum_{0 < l_1 < \dots < l_h} \Psi_{n_{t_1}, \dots, n_{t_2-1}}(l_1 \tau) \cdots \Psi_{n_{t_h}, \dots, n_r}(l_h \tau), \end{aligned} \quad (2.2)$$

where $0 < t_1 < \dots < t_h < r + 1$ describe the positions of \mathbf{y} 's in the word $w_1 \cdots w_r$, i.e.

$$w_1 \cdots w_r = \underbrace{\mathbf{x} \cdots \mathbf{x}}_{t_1-1} \mathbf{y} \underbrace{\mathbf{x} \cdots \mathbf{x}}_{t_2-t_1-1} \mathbf{y} \mathbf{x} \cdots \mathbf{y} \underbrace{\mathbf{x} \cdots \mathbf{x}}_{t_h-t_{h-1}-1} \mathbf{y} \underbrace{\mathbf{x} \cdots \mathbf{x}}_{r-t_h},$$

and $\zeta(n_1, \dots, n_{t_1-1}) = 1$ when $t_1 = 1$.

As we will use later, we remark that the above expression of words gives a one-to-one correspondence between words of length r in $\{\mathbf{x}, \mathbf{y}\}^*$ and the ordered subset of $\{1, 2, \dots, r\}$:

$$w_1 \cdots w_r \longleftrightarrow \{t_1, \dots, t_h\}, \quad (2.3)$$

where h is the number of \mathbf{y} 's in $w_1 \cdots w_r$. We remark that in the correspondence the word \mathbf{x}^r should correspond to the empty set as a subset of $\{1, 2, \dots, r\}$.

Proposition 2.2. *For integers $n_1, \dots, n_r \geq 2$, we have*

$$G_{n_1, \dots, n_r}(\tau) = \sum_{w_1, \dots, w_r \in \{\mathbf{x}, \mathbf{y}\}} G_{n_1, \dots, n_r}(w_1 \cdots w_r).$$

Proof. For $\lambda_1, \dots, \lambda_r \in \mathbb{Z}_L \tau + \mathbb{Z}_M$, the condition $0 \prec \lambda_1 \prec \dots \prec \lambda_r$ is by definition equivalent to $\lambda_i - \lambda_{i-1} \in P = P_{\mathbf{x}} \cup P_{\mathbf{y}}$ for all $1 \leq i \leq r-1$ (recall $\lambda_0 = 0$). Since $\lambda_i - \lambda_{i-1}$ can be either in $P_{\mathbf{x}}$ or in $P_{\mathbf{y}}$ we complete the proof. \square

Example. In the case of $r = 2$, one has for $n_1 \geq 2, n_2 \geq 3$

$$G_{n_1, n_2}(\tau) = \sum_{\substack{0 \prec \lambda_1 \prec \lambda_2 \\ \lambda_1, \lambda_2 \in \mathbb{Z}\tau + \mathbb{Z}}} \lambda_1^{-n_1} \lambda_2^{-n_2} = \sum_{\substack{\lambda_1 - \lambda_0 \in P \\ \lambda_2 - \lambda_1 \in P \\ \lambda_1, \lambda_2 \in \mathbb{Z}\tau + \mathbb{Z}}} \lambda_1^{-n_1} \lambda_2^{-n_2}$$

$$\begin{aligned}
 &= \left(\sum_{\substack{\lambda_1 - \lambda_0 \in P_{\mathbf{x}} \\ \lambda_2 - \lambda_1 \in P_{\mathbf{x}} \\ \lambda_1, \lambda_2 \in \mathbb{Z}\tau + \mathbb{Z}}} + \sum_{\substack{\lambda_1 - \lambda_0 \in P_{\mathbf{x}} \\ \lambda_2 - \lambda_1 \in P_{\mathbf{y}} \\ \lambda_1, \lambda_2 \in \mathbb{Z}\tau + \mathbb{Z}}} + \sum_{\substack{\lambda_1 - \lambda_0 \in P_{\mathbf{y}} \\ \lambda_2 - \lambda_1 \in P_{\mathbf{x}} \\ \lambda_1, \lambda_2 \in \mathbb{Z}\tau + \mathbb{Z}}} + \sum_{\substack{\lambda_1 - \lambda_0 \in P_{\mathbf{y}} \\ \lambda_2 - \lambda_1 \in P_{\mathbf{y}} \\ \lambda_1, \lambda_2 \in \mathbb{Z}\tau + \mathbb{Z}}} \right) \lambda_1^{-n_1} \lambda_2^{-n_2} \\
 &= G_{n_1, n_2}(\mathbf{xx}) + G_{n_1, n_2}(\mathbf{xy}) + G_{n_1, n_2}(\mathbf{yx}) + G_{n_1, n_2}(\mathbf{yy}).
 \end{aligned}$$

2.2 Computing the Fourier expansion

In this subsection, we give a Fourier expansion of $G_{n_1, \dots, n_r}(w_1 \cdots w_r)$.

Let us define the q -series $g_{n_1, \dots, n_r}(q)$ for integers $n_1, \dots, n_r \geq 1$ by

$$g_{n_1, \dots, n_r}(q) = \frac{(-2\pi\sqrt{-1})^{n_1 + \dots + n_r}}{(n_1 - 1)! \cdots (n_r - 1)!} \sum_{\substack{0 < u_1 < \dots < u_r \\ 0 < v_1, \dots, v_r}} v_1^{n_1 - 1} \cdots v_r^{n_r - 1} q^{u_1 v_1 + \dots + u_r v_r}, \quad (2.4)$$

which divided by $(-2\pi\sqrt{-1})^{n_1 + \dots + n_r}$ was studied in [2]. We remark that since $g_{n_1}(q)$ is the generating series of the divisor function $\sigma_{n_1-1}(n)$ up to a scalar factor, the coefficient of q^n in the q -series $g_{n_1, \dots, n_r}(q)$ can be regarded as a multiple version of the divisor sum:

$$\sigma_{n_1, \dots, n_r}(n) = \sum_{\substack{u_1 v_1 + \dots + u_r v_r = n \\ 0 < u_1 < \dots < u_r \\ v_1, \dots, v_r \in \mathbb{N}}} v_1^{n_1 - 1} \cdots v_r^{n_r - 1},$$

which is called the multiple divisor sum in [2] with the opposite convention (but we do not discuss their properties in this paper). We will investigate an algebraic structure related to the q -series $g_{n_1, \dots, n_r}(q)$ in a subsequent paper.

To give the Fourier expansion of $G_{n_1, \dots, n_r}(w_1, \dots, w_r)$, we need the following lemma.

Lemma 2.3. *For integers $n_1, \dots, n_r \geq 2$, we have*

$$\begin{aligned}
 &\sum_{q=1}^r \sum_{\substack{k_1 + \dots + k_r = n_1 + \dots + n_r \\ k_i \geq n_i, k_q = 1}} \left((-1)^{n_q + k_{q+1} + \dots + k_r} \prod_{\substack{j=1 \\ j \neq q}}^r \binom{k_j - 1}{n_j - 1} \right. \\
 &\quad \left. \times \zeta(k_{q-1}, k_{q-2}, \dots, k_1) \zeta(k_{q+1}, k_{q+2}, \dots, k_r) \right) = 0,
 \end{aligned}$$

where $\zeta(n_1, \dots, n_r) = 1$ when $r = 0$.

Proof. This was shown by using an iterated integral expression of multiple zeta values in [3, Section 5.5] (his notations $\mathcal{T}e^{n_r, \dots, n_1}(z)$ and $\mathcal{Z}e^{n_r, \dots, n_1}$ correspond to our $\Psi_{n_1, \dots, n_r}(z)$ and $\zeta(n_1, \dots, n_r)$, respectively). We remark that he proved the identities Lemma 2.3 for $n_1, \dots, n_r \geq 1$ with $n_1, n_r \geq 2$. \square

Proposition 2.4. *For integers $n_1, \dots, n_r \geq 2$ and a word $w_1 \cdots w_r \in \{\mathbf{x}, \mathbf{y}\}^*$ with the ordered subset $\{t_1, \dots, t_h\}$ given by the correspondence (2.3), we set $N_{t_m} = n_{t_m} + \cdots + n_{t_{m+1}-1}$ for $m \in \{1, \dots, h\}$ where $t_{h+1} = r + 1$. Then the function $G_{n_1, \dots, n_r}(w_1 \cdots w_r; \tau)$ has the following Fourier expansion:*

$$\begin{aligned} G_{n_1, \dots, n_r}(w_1 \cdots w_r) &= \zeta(n_1, \dots, n_{t_1-1}) \\ &\times \sum_{\substack{t_1 \leq q_1 \leq t_2-1 \\ t_2 \leq q_2 \leq t_3-1 \\ \vdots \\ t_h \leq q_h \leq r}} \sum_{\substack{k_{t_1} + \cdots + k_{t_2-1} = N_{t_1} \\ k_{t_2} + \cdots + k_{t_3-1} = N_{t_2} \\ \vdots \\ k_{t_h} + \cdots + k_r = N_{t_h} \\ k_{t_1}, k_{t_1+1}, \dots, k_r \geq 2}} \left\{ (-1)^{\sum_{m=1}^h (N_{t_m} + n_{q_m} + k_{q_m+1} + k_{q_m+2} + \cdots + k_{q_{m+1}-1})} \right. \\ &\times \left(\prod_{\substack{j=t_1 \\ j \neq q_1, \dots, q_h}}^r \binom{k_j-1}{n_j-1} \right) \left(\prod_{m=1}^h \zeta(\underbrace{k_{q_{m-1}}, \dots, k_{t_m}}_{q_m - t_m}) \zeta(\underbrace{k_{q_m+1}, \dots, k_{t_{m+1}-1}}_{t_{m+1} - q_m - 1}) \right) \\ &\times \left. g_{k_{q_1}, \dots, k_{q_h}}(q) \right\}, \end{aligned}$$

where $q = e^{2\pi\sqrt{-1}\tau}$, $\zeta(n_1, \dots, n_r) = g_{n_1, \dots, n_r}(q) = 1$ whenever $r = 0$ and $\prod_{\substack{j=t_1 \\ j \neq q_1, \dots, q_h}}^r \binom{k_j-1}{n_j-1} = 1$ when the product is empty, i.e. when $\{t_1, t_1+1, \dots, r\} = \{q_1, \dots, q_h\}$.

Proof. Put $N = n_1 + \cdots + n_r$. Using the partial fraction decomposition

$$\begin{aligned} &\frac{1}{(\tau + m_1)^{n_1} \cdots (\tau + m_r)^{n_r}} \\ &= \sum_{q=1}^r \sum_{\substack{k_1 + \cdots + k_r = N \\ k_1, \dots, k_r \geq 1}} \left(\prod_{j=1}^{q-1} \frac{\binom{k_j-1}{n_j-1}}{(m_q - m_j)^{k_j}} \right) \frac{(-1)^{N+n_q}}{(\tau + m_q)^{k_q}} \left(\prod_{j=q+1}^r \frac{(-1)^{k_j} \binom{k_j-1}{n_j-1}}{(m_j - m_q)^{k_j}} \right), \end{aligned}$$

we obtain

$$\begin{aligned} \Psi_{n_1, \dots, n_r}(\tau) &= \sum_{q=1}^r \sum_{\substack{k_1 + \dots + k_r = N \\ k_1, \dots, k_r \geq 1}} \left((-1)^{N+n_q+k_{q+1}+\dots+k_r} \prod_{\substack{j=1 \\ j \neq q}}^r \binom{k_j-1}{n_j-1} \right) \\ &\quad \times \zeta(\underbrace{k_{q-1}, k_{q-2}, \dots, k_1}_{q-1}) \Psi_{k_q}(\tau) \zeta(\underbrace{k_{q+1}, k_{q+2}, \dots, k_r}_{r-q}), \end{aligned} \quad (2.5)$$

where the implied interchange of order of summation is justified because the binomial coefficient $\binom{k_i-1}{n_i-1}$ vanishes if $k_i = 1$ or $n_i = 1$ and by Lemma 2.3 the coefficient of $\Psi_1(\tau)$ is zero. Using the Lipschitz formula (2.1) we easily obtain for integers $n_1, \dots, n_r \geq 2$

$$g_{n_1, \dots, n_r}(q) = \sum_{0 < u_1 < \dots < u_r} \Psi_{n_1}(u_1 \tau) \dots \Psi_{n_r}(u_r \tau). \quad (2.6)$$

Combining the above formulas with (2.2) we have the desired formula. \square

We remark that the formula (2.5), which in the case of $r = 2$ was done in [7, Proof of Theorem 6], is found in [3, Theorem 3] and holds when $n_1, \dots, n_r \geq 1$ with $n_1, n_r \geq 2$, but we use only the formula (2.5) for $n_1, \dots, n_r \geq 2$ in this paper.

We give an example which was carried out in [7]. From (2.2) and (2.6), it follows

$$\begin{aligned} G_{n_1, n_2}(\mathbf{xx}) &= \zeta(n_1, n_2), \\ G_{n_1, n_2}(\mathbf{xy}) &= \zeta(n_1) \sum_{0 < l} \Psi_{n_2}(l\tau) = \zeta(n_1) g_{n_2}(q), \\ G_{n_1, n_2}(\mathbf{yy}) &= \sum_{0 < l_1 < l_2} \Psi_{n_1}(l_1 \tau) \Psi_{n_2}(l_2 \tau) = g_{n_1, n_2}(q), \end{aligned}$$

and using (2.5), we have

$$G_{n_1, n_2}(\mathbf{yx}) = \sum_{0 < l} \Psi_{n_1, n_2}(l\tau) = \sum_{\substack{k_1 + k_2 = n_1 + n_2 \\ k_1, k_2 \geq 2}} \mathfrak{b}_{n_1, n_2}^{k_1} \zeta(k_1) g_{k_2}(q),$$

where for integers $n, n', k > 0$ we set

$$\mathfrak{b}_{n,n'}^k = (-1)^n \binom{k-1}{n-1} + (-1)^{k-n'} \binom{k-1}{n'-1}. \quad (2.7)$$

Thus the Fourier expansion of $G_{n_1, n_2}(\tau)$ is given by

$$G_{n_1, n_2}(\tau) = \zeta(n_1, n_2) + \sum_{\substack{k_1+k_2=n_1+n_2 \\ k_1, k_2 \geq 2}} (\delta_{n_1, k_1} + \mathfrak{b}_{n_1, n_2}^{k_1}) \zeta(k_1) g_{k_2}(q) + g_{n_1, n_2}(q), \quad (2.8)$$

where $\delta_{n,k}$ is the Kronecker delta.

3 The relationship between multiple Eisenstein series and the Goncharov coproduct

3.1 Regularised multiple zeta values

In this subsection, we recall the regularised multiple zeta value with respect to the shuffle product defined in [10]. We first recall an iterated integral expression of the multiple zeta value due to Kontsevich and Drinfel'd, and then introduce the algebraic setup of multiple zeta values given by Hoffman.

We denote by $\omega_0(t) = \frac{dt}{t}$ and $\omega_1(t) = \frac{dt}{1-t}$ holomorphic 1-forms on the smooth manifold $\mathbb{P}_{\mathbb{C}}^1 \setminus \{0, 1, \infty\}$. For integers $n_1, \dots, n_{r-1} \geq 1$ and $n_r \geq 2$ with $N = n_1 + \dots + n_r$, the multiple zeta value $\zeta(n_1, \dots, n_r)$ is expressible as an iterated integral on the smooth manifold $\mathbb{P}_{\mathbb{C}}^1 \setminus \{0, 1, \infty\}$:

$$\zeta(n_1, \dots, n_r) = \int_{0 < t_1 < t_2 < \dots < t_N < 1} \dots \int \omega_{a_1}(t_1) \wedge \omega_{a_2}(t_2) \wedge \dots \wedge \omega_{a_N}(t_N), \quad (3.1)$$

where $a_i = 1$ if $i \in \{1, n_1 + 1, n_1 + n_2 + 1, \dots, n_1 + \dots + n_{r-1} + 1\}$ and $a_i = 0$ otherwise.

Let $\mathfrak{H} = \mathbb{Q}\langle e_0, e_1 \rangle$ be the non-commutative polynomial algebra in two indeterminates e_0 and e_1 , and $\mathfrak{H}^1 := \mathbb{Q} + e_1 \mathfrak{H}$ and $\mathfrak{H}^0 := \mathbb{Q} + e_1 \mathfrak{H} e_0$ its

subalgebras. Set

$$y_n := e_1 e_0^{n-1} = e_1 \underbrace{e_0 \cdots e_0}_{n-1}$$

for each positive integer $n > 0$. It is easily seen that the subalgebra \mathfrak{H}^1 is freely generated by y_n 's ($n \geq 1$) as a non-commutative polynomial algebra:

$$\mathfrak{H}^1 = \mathbb{Q}\langle y_1, y_2, y_3, \dots \rangle.$$

We define the shuffle product, a \mathbb{Q} -bilinear product on \mathfrak{H} , inductively by

$$uw \mathbin{\boxplus} vw' = u(w \mathbin{\boxplus} vw') + v(uw \mathbin{\boxplus} w'),$$

with the initial condition $w \mathbin{\boxplus} 1 = 1 \mathbin{\boxplus} w = w$ ($1 \in \mathbb{Q}$), where $w, w' \in \mathfrak{H}$ and $u, v \in \{e_0, e_1\}$. This provides the structures of commutative \mathbb{Q} -algebras for spaces $\mathfrak{H}, \mathfrak{H}^1$ and \mathfrak{H}^0 (see [14]), which we denote by $\mathfrak{H}_{\boxplus}, \mathfrak{H}_{\boxplus}^1$ and $\mathfrak{H}_{\boxplus}^0$ respectively. By taking the iterated integral (3.1), with the identification $w_i(t) \leftrightarrow e_i$ ($i \in \{0, 1\}$), one can define an algebra homomorphism

$$\begin{aligned} Z : \mathfrak{H}_{\boxplus}^0 &\longrightarrow \mathbb{R} \\ y_{n_1} \cdots y_{n_r} &\longmapsto \zeta(n_1, \dots, n_r) \quad (n_r > 1) \end{aligned}$$

with $Z(1) = 1$, since it is known by K.T. Chen [5] that the iterated integral (3.1) satisfies the shuffle product formulas. By [10, Proposition 1], there is a \mathbb{Q} -algebra homomorphism

$$Z^{\boxplus} : \mathfrak{H}_{\boxplus}^1 \rightarrow \mathbb{R}[T]$$

which is uniquely determined by the properties that $Z^{\boxplus}|_{\mathfrak{H}_{\boxplus}^0} = Z$ and $Z^{\boxplus}(e_1) = T$. We note that the image of the word $y_{n_1} \cdots y_{n_r}$ in $\mathfrak{H}_{\boxplus}^1$ under the map Z^{\boxplus} is a polynomial in T whose coefficients are expressed as \mathbb{Q} -linear combinations of multiple zeta values.

Definition 3.1. *The regularised multiple zeta value, denoted by $\zeta^{\boxplus}(n_1, \dots, n_r)$, is defined as the constant term of $Z^{\boxplus}(y_{n_1} \cdots y_{n_r})$ in T :*

$$\zeta^{\boxplus}(n_1, \dots, n_r) := Z^{\boxplus}(y_{n_1} \cdots y_{n_r})|_{T=0}.$$

For example, we have $\zeta^{\text{m}}(2, 1) = -2\zeta(1, 2)$ and

$$\zeta^{\text{m}}(n_1, \dots, n_r) = \zeta(n_1, \dots, n_r) \quad (n_r \geq 2). \quad (3.2)$$

3.2 Hopf algebras of iterated integrals

In this subsection, we recall Hopf algebras of formal iterated integrals introduced by Goncharov.

In his paper [8, Section 2], Goncharov considered a formal version of the iterated integrals

$$\int_{a_0 < t_1 < t_2 < \dots < t_N < a_{N+1}} \dots \int \frac{dt_1}{t_1 - a_1} \wedge \frac{dt_2}{t_2 - a_2} \wedge \dots \wedge \frac{dt_N}{t_N - a_N} \quad (a_i \in \mathbb{C}). \quad (3.3)$$

He proved that the space $\mathcal{I}_\bullet(S)$ generated by formal iterated integrals carries a Hopf algebra structure. Let us recall the definition of the space $\mathcal{I}_\bullet(S)$.

Definition 3.2. *Let S be a set. Let us denote by $\mathcal{I}_\bullet(S)$ the commutative graded algebra over \mathbb{Q} generated by the set*

$$\{\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1}) \mid N \geq 0, a_i \in S\}.$$

The element $\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1})$ is homogeneous of degree N and involves the following relations.

- (I1) *For any $a, b \in S$, the unit is given by $\mathbb{I}(a; b) := \mathbb{I}(a; \emptyset; b) = 1$.*
- (I2) *The product is given by the shuffle product: for all integers $N, N' \geq 0$ and $a_i \in S$, one has*

$$\begin{aligned} & \mathbb{I}(a_0; a_1, \dots, a_N; a_{N+N'+1}) \mathbb{I}(a_0; a_{N+1}, \dots, a_{N+N'}; a_{N+N'+1}) \\ &= \sum_{\sigma \in \Sigma(N, N')} \mathbb{I}(a_0; a_{\sigma^{-1}(1)}, \dots, a_{\sigma^{-1}(N+N')}; a_{N+N'+1}), \end{aligned}$$

where $\Sigma(N, N')$ is the set of σ in the symmetric group $\mathfrak{S}_{N+N'}$ such that $\sigma(1) < \dots < \sigma(N)$ and $\sigma(N+1) < \dots < \sigma(N+N')$.

(I3) The path composition formula holds: for any $N \geq 0$ and $a_i, x \in S$, one has

$$\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1}) = \sum_{k=0}^N \mathbb{I}(a_0; a_1, \dots, a_k; x) \mathbb{I}(x; a_{k+1}, \dots, a_N; a_{N+1}).$$

(I4) For $N \geq 1$ and $a_i, a \in S$, $\mathbb{I}(a; a_1, \dots, a_N; a) = 0$.

We remark that the element $\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1})$ is an analogue of the iterated integral (3.3), since by K.T. Chen [5] iterated integrals satisfy (I1) to (I4) when the integral converges.

To give a Hopf algebra structure on the \mathbb{Q} -algebra $\mathcal{I}_\bullet(S)$, we define the coproduct on $\mathcal{I}_\bullet(S)$ by

$$\begin{aligned} & \Delta(\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1})) \\ &= \sum_{\substack{0 \leq k \leq N \\ i_0=0 < i_1 < \dots < i_k < i_{k+1}=N+1}} \prod_{p=0}^k \mathbb{I}(a_{i_p}; a_{i_{p+1}}, \dots, a_{i_{p+1}-1}; a_{i_{p+1}}) \\ & \quad \otimes \mathbb{I}(a_0; a_{i_1}, \dots, a_{i_k}; a_{N+1}), \end{aligned} \quad (3.4)$$

for any $N \geq 0$ and $a_i \in S$, and then extending by \mathbb{Q} -linearity. This is found in [8, Eq. (27)], with the factors interchanged, and is used in [4] (see Eq. (2.18)) as a coaction on the space of motivic multiple zeta values which we do not discuss in this paper.

Proposition 3.3. ([8, Proposition 2.2]) *The coproduct Δ gives $\mathcal{I}_\bullet(S)$ the structure of a commutative graded Hopf algebra, where the counit c is determined by the condition that it kills $\mathcal{I}_{>0}(S)$.*

We remark that the antipode A of the above Hopf algebra is uniquely and inductively determined by the definition. For example, since $\Delta(\mathbb{I}(a_0; a_1; a_2)) = \mathbb{I}(a_0; a_1; a_2) \otimes 1 + 1 \otimes \mathbb{I}(a_0; a_1; a_2)$ for any $a_0, a_1, a_2 \in S$, we have

$$A(\mathbb{I}(a_0; a_1; a_2)) + \mathbb{I}(a_0; a_1; a_2) = 0 = u \circ c(\mathbb{I}(a_0; a_1; a_2)),$$

where $u : \mathbb{Q} \rightarrow \mathcal{I}_\bullet(S)$ is the unit. We do not develop the precise formula for the antipode A in this paper.

3.3 Formal iterated integrals and regularised multiple zeta values

In this subsection, we define the map \mathfrak{z} described in the introduction. Hereafter, we consider only the Hopf algebra

$$\mathcal{I}_\bullet := \mathcal{I}_\bullet(S) \text{ with } S = \{0, 1\}.$$

Consider the quotient algebra

$$\mathcal{I}_\bullet^1 := \mathcal{I}_\bullet / \mathbb{I}(0; 0; 1)\mathcal{I}_\bullet.$$

It is easy to verify that $\mathbb{I}(0; 0; 1)$ is primitive, i.e. $\Delta(\mathbb{I}(0; 0; 1)) = 1 \otimes \mathbb{I}(0; 0; 1) + \mathbb{I}(0; 0; 1) \otimes 1$. Thus the ideal $\mathbb{I}(0; 0; 1)\mathcal{I}_\bullet$ generated by $\mathbb{I}(0; 0; 1)$ in the \mathbb{Q} -algebra \mathcal{I}_\bullet becomes a Hopf ideal, and hence the quotient map $\mathcal{I}_\bullet \rightarrow \mathcal{I}_\bullet^1$ induces a Hopf algebra structure on the quotient algebra \mathcal{I}_\bullet^1 . Let us denote by

$$I(a_0; a_1, \dots, a_N; a_{N+1}) \in \mathcal{I}_\bullet^1$$

an image of $\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1})$ in \mathcal{I}_\bullet^1 and by Δ the induced coproduct on \mathcal{I}_\bullet^1 given by the same formula as (3.4) replacing \mathbb{I} with I . As a result, we have the following proposition which we will use later.

Proposition 3.4. *The coproduct $\Delta : \mathcal{I}_\bullet^1 \rightarrow \mathcal{I}_\bullet^1 \otimes \mathcal{I}_\bullet^1$ is an algebra homomorphism, where the product on $\mathcal{I}_\bullet^1 \otimes \mathcal{I}_\bullet^1$ is defined in the standard way by $(w_1 \otimes w_2)(w'_1 \otimes w'_2) = w_1 w'_1 \otimes w_2 w'_2$ and the product on each summand \mathcal{I}_\bullet^1 .*

We remark that dividing \mathcal{I}_\bullet by $\mathbb{I}(0; 0; 1)\mathcal{I}_\bullet$ can be viewed as a regularisation for “ $\int_0^1 dt/t = -\log(0)$ ” which plays a role as $\mathbb{I}(0; 0; 1)$ in the evaluation of iterated integrals. For example, one can write $I(0; 0, 1, 0; 1) = -2I(0; 1, 0, 0; 1)$ in \mathcal{I}_\bullet^1 since it follows $\mathbb{I}(0; 0, 1, 0; 1) = \mathbb{I}(0; 0; 1)\mathbb{I}(0; 1, 0; 1) - 2\mathbb{I}(0; 1, 0, 0; 1)$, and this computation corresponds to taking the constant term of $\int_\varepsilon^1 \frac{dt_1}{t_1} \int_\varepsilon^{t_1} \frac{dt_2}{1-t_2} \int_\varepsilon^{t_2} \frac{dt_3}{t_3}$ as a polynomial of $\log(\varepsilon)$ and letting $\varepsilon \rightarrow 0$.

By the standard calculation about the shuffle product formulas, we obtain more identities in the space \mathcal{I}_\bullet^1 (see [4, p.955]).

1. For $n \geq 1$ and $a, b \in \{0, 1\}$, we have

$$I(a; \underbrace{0, \dots, 0}_n; b) = 0. \quad (3.5)$$

2. For integers $n \geq 0, n_1, \dots, n_r \geq 1$, we have

$$\begin{aligned} & I(0; \underbrace{0, \dots, 0}_n, \underbrace{1, 0, \dots, 0}_{n_1}, \dots, \underbrace{1, 0, \dots, 0}_{n_r}; 1) \\ &= (-1)^n \sum_{\substack{k_1 + \dots + k_r = n_1 + \dots + n_r + n \\ k_1, \dots, k_r \geq 1}} \left(\prod_{j=1}^r \binom{k_j - 1}{n_j - 1} \right) I(k_1, \dots, k_r), \end{aligned} \quad (3.6)$$

where we set

$$I(n_1, \dots, n_r) := I(0; \underbrace{1, 0, \dots, 0}_{n_1}, \dots, \underbrace{1, 0, \dots, 0}_{n_r}; 1).$$

In order to define the map \mathfrak{J}^m as a \mathbb{Q} -linear map, we give a linear basis of the space \mathcal{I}_\bullet^1 .

Proposition 3.5. *The set of elements $\{I(n_1, \dots, n_r) \mid r \geq 0, n_i \geq 1\}$ is a linear basis of the space \mathcal{I}_\bullet^1 .*

Proof. Recall the result of Goncharov [8, Proposition 2.1]: for each integer $N \geq 0$ and $a_0, \dots, a_{N+1} \in \{0, 1\}$ one has

$$\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1}) = (-1)^N \mathbb{I}(a_{N+1}; a_N, \dots, a_1; a_0), \quad (3.7)$$

which essentially follows from (I3) and (I4). Then, we find that the collection

$$\{\mathbb{I}(0; a_1, \dots, a_N; 1) \mid N \geq 0, a_i \in \{0, 1\}\}$$

forms a linear basis of the linear space \mathcal{I}_\bullet , since none of the relations (I1) to (I4) yield \mathbb{Q} -linear relations among them. Combining this with (3.6), we obtain the desired basis. \square

Let $\mathfrak{z}^{\text{III}} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{R}$ be the \mathbb{Q} -linear map given by

$$\begin{aligned} \mathfrak{z}^{\text{III}} : \mathcal{I}_{\bullet}^1 &\longrightarrow \mathbb{R} \\ I(n_1, \dots, n_r) &\longmapsto \zeta^{\text{III}}(n_1, \dots, n_r) \end{aligned}$$

and $\mathfrak{z}^{\text{III}}(1) = 1$.

Proposition 3.6. *The map $\mathfrak{z}^{\text{III}} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{R}$ is an algebra homomorphism.*

Proof. By Proposition 3.5, we find that the \mathbb{Q} -linear map $\mathfrak{H}_{\text{III}}^1 \rightarrow \mathcal{I}_{\bullet}^1$ given by $e_{a_1} \cdots e_{a_N} \mapsto I(0; a_1, \dots, a_N; 1)$ is an isomorphism between \mathbb{Q} -algebras. Then the result follows from the standard fact that the map $Z^{\text{III}}|_{T=0} : \mathfrak{H}_{\text{III}}^1 \rightarrow \mathbb{R}$ given by $y_{n_1} \cdots y_{n_r} \mapsto \zeta^{\text{III}}(n_1, \dots, n_r)$ is an algebra homomorphism. \square

3.4 Computing the Goncharov coproduct

In this subsection, we express a formula for the Goncharov coproduct Δ for $I(n_1, \dots, n_r)$ as certain algebraic combinations of $I(k_1, \dots, k_i)$'s. Although the formula can be obtained from Propositions 3.7 and 3.9, we do not give a closed formula for $\Delta(I(n_1, \dots, n_r))$ in general. We present a closed formula for only $\Delta(I(n_1, n_2, n_3))$ in the end of this subsection.

To describe the formula, it is convenient to use the algebraic setup. Let $\mathfrak{H}' := \langle e_0, e_1, e'_0, e'_1 \rangle$ be the non-commutative polynomial algebra in four indeterminates e_0, e_1, e'_0 and e'_1 . For integers $0 < i_1 < i_2 < \cdots < i_k < N+1$ ($0 \leq k \leq N$), the word of length N in \mathfrak{H}' marking only letters $e_{a_{i_1}}, e_{a_{i_2}}, \dots, e_{a_{i_k}}$ with a prime symbol is denoted by $\mathbf{e}_{i_1, \dots, i_k}(a_1, \dots, a_N)$:

$$\mathbf{e}_{i_1, \dots, i_k}(a_1, \dots, a_N) := e_{a_1} \cdots e_{a_{i_1-1}} \left(\prod_{p=1}^{k-1} e'_{a_{i_p}} e_{a_{i_{p+1}}} \cdots e_{a_{i_{p+1}-1}} \right) e'_{a_{i_k}} e_{a_{i_k+1}} \cdots e_{a_N},$$

where the product $\prod_{p=1}^{k-1}$ means the concatenation product. Let $\varphi : \mathfrak{H}' \rightarrow \mathcal{I}_{\bullet}^1 \otimes \mathcal{I}_{\bullet}^1$ be the \mathbb{Q} -linear map that assigns to each word $\mathbf{e}_{i_1, \dots, i_k}(a_1, \dots, a_N)$

the right-hand side factor of the equation (3.4) with $a_0 = 0$ and $a_{N+1} = 1$:

$$\begin{aligned} & \varphi(\mathbf{e}_{i_1, \dots, i_k}(a_1, \dots, a_N)) \\ &= \prod_{p=0}^k I(a_{i_p}; a_{i_{p+1}}, \dots, a_{i_{p+1}-1}; a_{i_{p+1}}) \otimes I(0; a_{i_1}, \dots, a_{i_k}; 1), \end{aligned}$$

where we set $a_{i_0} = 0$ and $a_{i_{k+1}} = 1$. For example, we have $\varphi(\mathbf{e}_{2,3}(a_1, \dots, a_4)) = \varphi(e_{a_1} e'_{a_2} e'_{a_3} e_{a_4}) = I(0; a_1; a_2) I(a_2; a_3) I(a_3; a_4; 1) \otimes I(0; a_2, a_3; 1)$.

In the rest of this subsection, for integers $n_1, \dots, n_r \geq 1$ with $N = n_1 + \dots + n_r$, we set

$$\{a_1, \dots, a_N\} = \{1, \underbrace{0, \dots, 0}_{n_1-1}, \dots, 1, \underbrace{0, \dots, 0}_{n_r-1}\},$$

and write $\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r) := \mathbf{e}_{i_1, \dots, i_k}(a_1, \dots, a_N)$. Let S_{n_1, \dots, n_r}^1 be the set of positions of 1's:

$$S_{n_1, \dots, n_r}^1 := \{1, n_1 + 1, \dots, n_1 + \dots + n_{r-1} + 1\}.$$

Then $a_j = 1$ if j lies in the set S_{n_1, \dots, n_r}^1 and $a_j = 0$ otherwise. Using these notations, one has

$$\Delta(I(n_1, \dots, n_r)) = \sum_{k=0}^N \sum_{0 < i_1 < \dots < i_k < N+1} \varphi(\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r)). \quad (3.8)$$

To compute (3.8), we split the right-hand side of (3.8) into 2^r sums of certain terms. For this, we need the following correspondence.

For each word $w_1 \cdots w_r$ of length r in $\{\mathbf{x}, \mathbf{y}\}^*$, we can obtain a unique ordered subset $\{j_1, \dots, j_h\} \subset S_{n_1, \dots, n_r}^1$ via the following correspondences:

$$w_1 \cdots w_r \longleftrightarrow \{t_1, \dots, t_h\} \longleftrightarrow \{j_1, \dots, j_h\}, \quad (3.9)$$

where the first correspondence is given by the correspondence (2.3) and the second one is simply given by $1 \leftrightarrow 1, n_1 + 1 \leftrightarrow 2, \dots, n_1 + \dots + n_{r-1} + 1 \leftrightarrow r$ (note that the number h corresponds to the number of \mathbf{y} 's in $w_1 \cdots w_r$). For

instance, the word \mathbf{yxyx}^{r-3} corresponds to the ordered subset $\{1, n_1 + n_2 + 1\} \subset S_{n_1, \dots, n_r}^1$. We note that the word \mathbf{x}^r corresponds to the empty set as a subset of S_{n_1, \dots, n_r}^1 .

For integers $n_1, \dots, n_r \geq 1$ and a word $w_1 \cdots w_r$ ($w_i \in \{\mathbf{x}, \mathbf{y}\}$) with the ordered subset $\{j_1, \dots, j_h\}$ given by the correspondence (3.9), we let

$$\psi_{n_1, \dots, n_r}(w_1 \cdots w_r) := \sum_{k=h}^N \sum_{\substack{0 < i_1 < \dots < i_k < N+1 \\ \#\{i_1, \dots, i_k\} \cap S_{n_1, \dots, n_r}^1 = \{j_1, \dots, j_h\}}} \varphi(\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r)). \quad (3.10)$$

Proposition 3.7. *For integers $n_1, \dots, n_r \geq 1$, we have*

$$\Delta(I(n_1, \dots, n_r)) = \sum_{w_1, \dots, w_r \in \{\mathbf{x}, \mathbf{y}\}} \psi_{n_1, \dots, n_r}(w_1 \cdots w_r).$$

Proof. For the word $\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r)$, we denote by h the number of e'_1 's in the prime symbols $e'_{a_{i_1}}, \dots, e'_{a_{i_k}}$, i.e. $h = \deg_{e'_1}(\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r))$. Since $a_j = 1$ if and only if $j \in S_{n_1, \dots, n_r}^1$, we have $h = \#\(\{i_1, \dots, i_k\} \cap S_{n_1, \dots, n_r}^1)$. We notice that h can be chosen from $\{0, 1, \dots, \min\{r, k\}\}$ for each k . Then, the formula (3.8) can be written in the form

$$\begin{aligned} (3.8) &= \sum_{k=0}^N \sum_{h=0}^{\min\{r, k\}} \sum_{\substack{0 < i_1 < \dots < i_k < N+1 \\ \#\{i_1, \dots, i_k\} \cap S_{n_1, \dots, n_r}^1 = h}} \varphi(\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r)) \\ &= \sum_{h=0}^r \sum_{k=h}^N \sum_{\substack{0 < i_1 < \dots < i_k < N+1 \\ \#\{i_1, \dots, i_k\} \cap S_{n_1, \dots, n_r}^1 = h}} \varphi(\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r)). \end{aligned}$$

By specifying the ordered subset of S_{n_1, \dots, n_r}^1 with length h , the above third sum can be split into the following sums:

$$(3.8) = \sum_{h=0}^r \sum_{k=h}^N \sum_{\substack{\{j_1, \dots, j_h\} \subset S_{n_1, \dots, n_r}^1 \\ j_1 < \dots < j_h}} \sum_{\substack{0 < i_1 < \dots < i_k < N+1 \\ \{i_1, \dots, i_k\} \cap S_{n_1, \dots, n_r}^1 = \{j_1, \dots, j_h\}}} \varphi(\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r))$$

$$\begin{aligned}
 &= \sum_{h=0}^r \sum_{\substack{\{j_1, \dots, j_h\} \subset S_{n_1, \dots, n_r}^1 \\ j_1 < \dots < j_h}} \sum_{k=h}^N \sum_{\substack{0 < i_1 < \dots < i_k < N+1 \\ \{i_1, \dots, i_k\} \cap S_{n_1, \dots, n_r}^1 = \{j_1, \dots, j_h\}}} \varphi(\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r)) \\
 &= \sum_{h=0}^r \sum_{\substack{w_1, \dots, w_r \in \{\mathbf{x}, \mathbf{y}\} \\ \#\{l | w_l = \mathbf{y}, 1 \leq l \leq r\} = h}} \psi_{n_1, \dots, n_r}(w_1 \cdots w_r) \\
 &= \sum_{w_1, \dots, w_r \in \{\mathbf{x}, \mathbf{y}\}} \psi_{n_1, \dots, n_r}(w_1 \cdots w_r),
 \end{aligned}$$

which completes the proof. \square

We express (3.10) as algebraic combinations of $I(k_1, \dots, k_i)$'s. To do this, we extract possible nonzero terms from the right-hand side of (3.10) by using (I4). For a positive integer n , we define $\eta_0(n)$ as the sum of all words of degree $n - 1$ consisting of e_0 and a consecutive e'_0 :

$$\eta_0(n) = \sum_{\substack{\alpha + k + \beta = n \\ \alpha, \beta \geq 0 \\ k \geq 1}} e_0^\alpha (e'_0)^{k-1} e_0^\beta.$$

Proposition 3.8. *For integers $n_1, \dots, n_r \geq 1$ and a word $w_1 \cdots w_r$ of length r in $\{\mathbf{x}, \mathbf{y}\}^*$ with the ordered subset $\{t_1, \dots, t_h\}$ given by the correspondence (2.3), we have*

$$\begin{aligned}
 \psi_{n_1, \dots, n_r}(w_1 \cdots w_r) &= \sum_{\substack{t_1 \leq q_1 \leq t_2 - 1 \\ t_2 \leq q_2 \leq t_3 - 1 \\ \vdots \\ t_h \leq q_h \leq r}} \\
 &\varphi\left(y_{n_1} \cdots y_{n_{t_1-1}} \prod_{m=1}^h \underbrace{\left(e'_0 e_0^{n_{t_m}-1} y_{n_{t_m+1}} \cdots y_{n_{q_m-1}} e_1 \eta_0(n_{q_m}) y_{n_{q_m+1}} \cdots y_{n_{t_{m+1}-1}\right)}_{\text{degree in } e_1 = q_m - t_m}\right),
 \end{aligned}$$

where $t_{h+1} = r + 1$ and the product $\prod_{m=1}^h$ means the concatenation product of words.

Proof. It follows $\psi_{n_1, \dots, n_r}(\mathbf{x}^r) = \varphi(y_{n_1} \cdots y_{n_r})$, so we consider the case $h > 0$

which means the number of \mathbf{y} 's in $w_1 \cdots w_r$ is greater than 0. We note that the sum defining (3.10) runs over all words $c_{a_1} \cdots c_{a_N}$ ($c_{a_i} \in \{e_{a_i}, e'_{a_i}\}$) with k ($h \leq k \leq N$) prime symbols whose positions of e'_1 's are placed on the ordered subset $\{j_1, \dots, j_h\}$ of S_{n_1, \dots, n_r}^1 corresponding to the word $w_1 \cdots w_r$ via (3.9):

$$(3.10) = \sum_{k=h}^N \sum_{\substack{w_0, w_1, \dots, w_h \in \{e_0, e_1, e'_0\}^* \\ \deg_{e'_0}(w_0 w_1 \cdots w_h) = k-h \\ \deg(w_0) = j_1 - 1 \\ \deg(e'_1 w_m) = j_{m+1} - j_m \quad (1 \leq m \leq h) \\ j_{h+1} = N+1}} \varphi\left(w_0 \prod_{m=1}^h (e'_1 w_m)\right).$$

We find by (I4) that $\varphi(\mathbf{e}_{i_1, \dots, i_k}(n_1, \dots, n_r))$ is 0 whenever $a_{i_1} = 0$ (notice $a_0 = 0, a_1 = 1$). This implies that if the above w_0 's degree in the letter e'_0 is greater than 0, then $\varphi\left(w_0 \prod_{m=1}^h (e'_1 w_m)\right) = 0$. For a word $w \in \mathfrak{S}'$, we also find $\varphi(w) = 0$ if w has a subword of the form $e'_0 v e'_0$ with $v \in \mathfrak{S}$ ($v \neq \emptyset$), i.e. $w = w_1 e'_0 v e'_0 w_2$ for some $w_1, w_2 \in \mathfrak{S}'$, because the left-hand side factor of $\varphi(w)$ involves $I(0; v; 0)$ which by (I4) is 0. This implies that the above second sum regarding to w_m ($1 \leq m \leq h$) of the form $w_m = w_1 e'_0 v e'_0 w_2$ with $v \in \{e_0, e_1\}^*$ ($v \neq \emptyset$) and $w_1, w_2 \in \{e_0, e_1, e'_0\}^*$ can be excluded. Thus, the possible nonzero terms in (3.10), sieved out by (I4), occur if $w_0 = y_{n_1} \cdots y_{n_{t_1-1}}$ and w_m is written in the form

$$\underbrace{e_0^{n_{t_m}-1} y_{n_{t_m+1}} \cdots y_{n_{q_m-1}} e_1 e_0^\alpha (e'_0)^k e_0^\beta y_{n_{q_m+1}} \cdots y_{n_{t_{m+1}-1}}}_{\text{degree in } e_1 = q_m - t_m},$$

where $q_m \in \{t_m, t_m + 1, \dots, t_{m+1} - 1\}$, $\alpha, \beta, k \in \mathbb{Z}_{\geq 0}$ with $\alpha + k + \beta = n_{q_m} - 1$ and $\{t_1, \dots, t_h\}$ corresponds to the word $w_1 \cdots w_r$ given by (2.3). This completes the proof. \square

Before giving an explicit formula for $\psi_{n_1, \dots, n_r}(w_1 \cdots w_r)$, we illustrate an example for $r = 2$. It follows $\psi_{n_1, n_2}(\mathbf{xx}) = \varphi(e_1 e_0^{n_1-1} e_1 e_0^{n_2-1}) = I(n_1, n_2) \otimes 1$. By (3.5) one can compute

$$\psi_{n_1, n_2}(\mathbf{xy}) = \sum_{\substack{\alpha+k+\beta=n_2 \\ \alpha, \beta \geq 0 \\ k \geq 1}} \varphi(e_1 e_0^{n_1-1} e'_1 e_0^\alpha (e'_0)^{k-1} e_0^\beta) = I(n_1) \otimes I(n_2),$$

$$\begin{aligned}\psi_{n_1, n_2}(\mathbf{y}\mathbf{y}) &= \sum_{\substack{\alpha_1+k_1+\beta_1=n_1 \\ \alpha_1, \beta_1 \geq 0 \\ k_1 \geq 1}} \sum_{\substack{\alpha_2+k_2+\beta_2=n_2 \\ \alpha_2, \beta_2 \geq 0 \\ k_2 \geq 1}} \varphi(e'_1 e_0^{\alpha_1} (e'_0)^{k_1-1} e_0^{\beta_1} e'_1 e_0^{\alpha_2} (e'_0)^{k_2-1} e_0^{\beta_2}) \\ &= 1 \otimes I(n_1, n_2),\end{aligned}$$

and using (3.7) and (3.6) we have

$$\begin{aligned}\psi_{n_1, n_2}(\mathbf{y}\mathbf{x}) &= \sum_{\substack{\alpha+k+\beta=n_1 \\ \alpha, \beta \geq 0 \\ k \geq 1}} \varphi(e'_1 e_0^\alpha (e'_0)^{k-1} e_0^\beta e_1 e_0^{n_2-1}) + \sum_{\substack{\alpha+k+\beta=n_2 \\ \alpha, \beta \geq 0 \\ k \geq 1}} \varphi(e'_1 e_0^{n_1-1} e_1 e_0^\alpha (e'_0)^{k-1} e_0^\beta) \\ &= \sum_{\substack{k_1+k_2=n_1+n_2 \\ k_1, k_2 \geq 1}} \mathbf{b}_{n_1, n_2}^{k_1} I(k_1) \otimes I(k_2),\end{aligned}$$

where $\mathbf{b}_{n, n'}$ is defined in (2.7). Therefore by Proposition 3.7 we have

$$\begin{aligned}\Delta(I(n_1, n_2)) &= I(n_1, n_2) \otimes 1 + \sum_{\substack{k_1+k_2=n_1+n_2 \\ k_1, k_2 \geq 1}} (\delta_{n_1, k_1} + \mathbf{b}_{n_1, n_2}^{k_1}) I(k_1) \otimes I(k_2) + 1 \otimes I(n_1, n_2).\end{aligned}\tag{3.11}$$

Proposition 3.9. *For integers $n_1, \dots, n_r \geq 2$ and a word $w_1 \cdots w_r \in \{\mathbf{x}, \mathbf{y}\}^*$ with the ordered subset $\{t_1, \dots, t_h\}$ given by the correspondence (2.3), we set $N_{t_m} = n_{t_m} + \cdots + n_{t_{m+1}-1}$ for $m \in \{1, \dots, h\}$ where $t_{h+1} = r+1$. Then we have*

$$\begin{aligned}\psi_{n_1, \dots, n_r}(w_1 \cdots w_r) &= (I(n_1, \dots, n_{t_1-1}) \otimes 1) \\ &\times \sum_{\substack{t_1 \leq q_1 \leq t_2-1 \\ t_2 \leq q_2 \leq t_3-1 \\ \vdots \\ t_h \leq q_h \leq r}} \sum_{\substack{k_{t_1} + \cdots + k_{t_2-1} = N_{t_1} \\ k_{t_2} + \cdots + k_{t_3-1} = N_{t_2} \\ \vdots \\ k_{t_h} + \cdots + k_r = N_{t_h} \\ k_i \geq 1}} \left\{ (-1)^{\sum_{m=1}^h (N_{t_m} + n_{q_m} + k_{q_m+1} + k_{q_m+2} + \cdots + k_{q_{m+1}-1})} \right. \\ &\times \left(\prod_{\substack{j=t_1 \\ j \neq q_1, \dots, q_h}}^r \binom{k_j-1}{n_j-1} \right) \left(\prod_{m=1}^h \underbrace{I(k_{q_m-1}, \dots, k_{t_m})}_{q_m-t_m} \underbrace{I(k_{q_m+1}, \dots, k_{t_{m+1}-1})}_{t_{m+1}-q_m-1} \right)\end{aligned}$$

$$\otimes I(k_{q_1}, \dots, k_{q_h}) \Big\},$$

where $\prod_{\substack{j=t_1 \\ j \neq q_1, \dots, q_h}}^r \binom{k_j-1}{n_j-1} = 1$ when $\{t_1, t_1+1, \dots, r\} = \{q_1, \dots, q_h\}$.

Proof. This can be verified by applying the identities (3.7), (3.5) and (3.6) to the formula in Proposition 3.8. \square

For the future literature, we present an explicit formula for $\Delta(I(n_1, n_2, n_3))$ obtained from Propositions 3.7 and 3.9:

$$\begin{aligned} & \Delta(I(n_1, n_2, n_3)) \\ &= I(n_1, n_2, n_3) \otimes 1 + I(n_1, n_2) \otimes I(n_3) + I(n_1) \otimes I(n_2, n_3) + 1 \otimes I(n_1, n_2, n_3) \\ &+ \sum_{\substack{k_1+k_2+k_3=n_1+n_2+n_3 \\ k_1, k_2, k_3 \geq 1}} \left\{ (\delta_{n_3, k_3} \mathbf{b}_{n_1, n_2}^{k_1} + \delta_{n_1, k_2} \mathbf{b}_{n_2, n_3}^{k_1}) I(k_1) \otimes I(k_2, k_3) \right. \\ &+ \left((-1)^{n_1+k_3} \binom{k_2-1}{n_3-1} + (-1)^{n_1+n_2} \binom{k_2-1}{n_1-1} \right) \binom{k_1-1}{n_2-1} I(k_1, k_2) \otimes I(k_3) \\ &+ \left. \left((-1)^{n_1+n_3+k_2} \binom{k_1-1}{n_1-1} \binom{k_2-1}{n_3-1} + \delta_{k_1, n_1} \mathbf{b}_{n_2, n_3}^{k_2} \right) I(k_1) I(k_2) \otimes I(k_3) \right\}. \end{aligned}$$

3.5 Proof of Theorem 1.1

We now give a proof of Theorem 1.1. Recall the q -series $g_{n_1, \dots, n_r}(q)$ defined in (2.4). Let $\mathfrak{g} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{C}[[q]]$ be the \mathbb{Q} -linear map given by $\mathfrak{g}(I(n_1, \dots, n_r)) = g_{n_1, \dots, n_r}(q)$ and $\mathfrak{g}(1) = 1$.

Proof of Theorem 1.1. Taking $\mathfrak{z}^{\text{III}} \otimes \mathfrak{g}$ for the explicit formula in Proposition 3.9 and comparing this with Proposition 2.4, we have

$$(\mathfrak{z}^{\text{III}} \otimes \mathfrak{g})(\psi_{n_1, \dots, n_r}(w_1 \cdots w_r)) = G_{n_1, \dots, n_r}(w_1 \cdots w_r).$$

Here the second sum (relating to k_i) of the formula in Proposition 3.9 differs from that of the formula in Proposition 2.4, but apparently it is the same because binomial coefficient terms allow us to take $k_i \geq n_i$ for $t_1 \leq i \leq r$ without $i = q_1, \dots, q_h$, and by Lemma 2.3 it turns out that the coefficient

of $g_{k_{q_1}, \dots, k_{q_h}}(q)$ becomes 0 if $k_{q_j} = 1$ for some $1 \leq j \leq h$. With this the statement follows from Propositions 2.2 and 3.7. \square

We remark that the binomial coefficients in Proposition 3.9 essentially arise from the formula (3.6) obtained from the shuffle product (I2), and the binomial coefficients in Proposition 2.4 are caused by the partial fraction decomposition. Thus a well-known similarity between the shuffle product (I2) and the partial fraction decomposition is an only exposition of Theorem 1.1 so far.

4 The algebra of multiple Eisenstein series

4.1 The algebra of the generating series of the multiple divisor sum

In this subsection, we construct the algebra homomorphism $\mathfrak{g}^{\text{III}} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{C}[[q]]$ described in the introduction.

We give an expression of the generating function of $g_{n_1, \dots, n_r}(q)$ as an iterated multiple sum. We let

$$g(x_1, \dots, x_r) = \sum_{n_1, \dots, n_r \geq 1} \frac{g_{n_1, \dots, n_r}(q)}{(-2\pi\sqrt{-1})^{n_1 + \dots + n_r}} x_1^{n_1-1} \dots x_r^{n_r-1},$$

and set

$$H_{(x_1, \dots, x_r)}^{(n_1, \dots, n_r)} = \sum_{0 < u_1 < \dots < u_r} e^{u_1 x_1} \left(\frac{q^{u_1}}{1 - q^{u_1}} \right)^{n_1} \dots e^{u_r x_r} \left(\frac{q^{u_r}}{1 - q^{u_r}} \right)^{n_r},$$

where n_1, \dots, n_r are positive integers and x_1, \dots, x_r are commutative variables, i.e. these are elements in the power series ring $\mathcal{K}[[x_1, \dots, x_r]]$, where $\mathcal{K} = \mathbb{Q}[[q]]$.

Proposition 4.1. *For each integer $r > 0$ we have*

$$g(x_1, \dots, x_r) = H_{(x_r - x_{r-1}, \dots, x_2 - x_1, x_1)}^{(1, \dots, 1, 1)}.$$

Proof. When $r = 2$ this was computed in the proof of Theorem 7 in [7] with the opposite convention. Its generalisation is easy and omitted. \square

We easily find that the power series $H\binom{n_1, \dots, n_r}{x_1, \dots, x_r}$ satisfies the harmonic product. More precisely, for a set X let us denote by $\mathfrak{H}(X)$ the non-commutative polynomial algebra over \mathbb{Q} generated by non-commutative symbols $\binom{n_1, \dots, n_r}{z_1, \dots, z_r}$ indexed by $n_1, \dots, n_r \in \mathbb{N}$ and $z_1, \dots, z_r \in X_{\mathbb{Z}}$, where $X_{\mathbb{Z}}$ is the set of finite sums of the elements in X . The concatenation product is given by $\binom{n_1, \dots, n_r}{z_1, \dots, z_r} \cdot \binom{n_{r+1}, \dots, n_{r+s}}{z_{r+1}, \dots, z_{r+s}} = \binom{n_1, \dots, n_r, n_{r+1}, \dots, n_{r+s}}{z_1, \dots, z_r, z_{r+1}, \dots, z_{r+s}}$. As usual, the harmonic product $*$ on $\mathfrak{H}(X)$ is inductively defined for $n, n' \in \mathbb{N}$, $z, z' \in X_{\mathbb{Z}}$ and words w, w' in $\mathfrak{H}(X)$ by

$$\begin{aligned} & \binom{(n)}{(z)} \cdot w * \binom{(n')}{(z')} \cdot w' \\ &= \binom{(n)}{(z)} \cdot (w * \binom{(n')}{(z')} \cdot w') + \binom{(n')}{(z')} \cdot (\binom{(n)}{(z)} \cdot w) * w' + \binom{(n+n')}{(z+z')} \cdot (w * w'), \end{aligned}$$

with the initial condition $w * 1 = 1 * w = w$. Then the \mathbb{Q} -linear map H defined by

$$\begin{aligned} H : \mathfrak{H}(\{x_i\}_{i=1}^{\infty}) &\longrightarrow \mathcal{R} := \varinjlim \mathcal{K}[[x_1, \dots, x_r]] \\ \binom{(n_1, \dots, n_r)}{(x_{i_1}, \dots, x_{i_r})} &\longmapsto H\binom{(n_1, \dots, n_r)}{(x_{i_1}, \dots, x_{i_r})} \end{aligned}$$

becomes an algebra homomorphism of commutative \mathbb{Q} -algebras.

It is known by Hoffman [9, Theorem 2.5] that there is an explicit isomorphism between algebras with respect to the harmonic product and the shuffle product. This isomorphism is denoted by $\exp : \mathfrak{H}_{\text{m}}(X) \rightarrow \mathfrak{H}_{*}(X)$, called the exponential map (see [9, p.52]), where $\mathfrak{H}_{\circ}(X)$ is the algebra equipped with the product $\circ = *$ or m (the shuffle product on $\mathfrak{H}(X)$ is defined in the same way as in m on $\mathfrak{H} = \mathbb{Q}\langle e_0, e_1 \rangle$, switching the underlying vector space to $\mathfrak{H}(X)$). As a consequence, we have the following proposition.

Proposition 4.2. *The composition map $H \circ \exp$ is an algebra homomorphism:*

$$H \circ \exp : \mathfrak{H}_{\text{m}}(\{x_i\}_{i=1}^{\infty}) \rightarrow \mathcal{R}.$$

We use this map to obtain the q -series satisfying the shuffle product formulas.

Before going to the general case, we illustrate this procedure for $r = 2$. We let $h(x_1, x_2) := H \circ \exp\left(\begin{smallmatrix} 1,1 \\ x_1, x_2 \end{smallmatrix}\right) = H\left(\begin{smallmatrix} 1,1 \\ x_1, x_2 \end{smallmatrix}\right) + \frac{1}{2}H\left(\begin{smallmatrix} 2 \\ x_1+x_2 \end{smallmatrix}\right)$. By Proposition 4.2, the harmonic product of H 's gives rise to the shuffle product of h 's: $H\left(\begin{smallmatrix} 1 \\ x_1 \end{smallmatrix}\right)H\left(\begin{smallmatrix} 1 \\ x_2 \end{smallmatrix}\right) = h(x_1, x_2) + h(x_2, x_1)$. Modelling the change of variables used in Proposition 4.1, set $g_{\text{m}}(x_1, x_2) := h(x_2 - x_1, x_1) = g(x_1, x_2) + \frac{1}{2}H\left(\begin{smallmatrix} 2 \\ x_2 \end{smallmatrix}\right)$. Then, we get $g(x_1)g(x_2) = H\left(\begin{smallmatrix} 1 \\ x_1 \end{smallmatrix}\right)H\left(\begin{smallmatrix} 1 \\ x_2 \end{smallmatrix}\right) = g_{\text{m}}(x_2, x_1 + x_2) + g_{\text{m}}(x_1, x_1 + x_2)$, which shows that the coefficients of $g_{\text{m}}(x_1, x_2)$ satisfy the shuffle product (I2) (note that the shuffle product formula (I2) gives $I(n_1)I(n_2) = \sum_{k_1+k_2=n_1+n_2} \left(\binom{k_2-1}{n_1-1} + \binom{k_2-1}{n_2-1}\right)I(k_1, k_2)$).

We remark that the above shuffle relation provides the following relation:

$$g(x_1)g(x_2) = g(x_2, x_1 + x_2) + g(x_1, x_1 + x_2) + H\left(\begin{smallmatrix} 2 \\ x_1+x_2 \end{smallmatrix}\right). \quad (4.1)$$

Since $H\left(\begin{smallmatrix} 2 \\ x_1+x_2 \end{smallmatrix}\right) \neq 0$, this proves that the q -series $g_{n_1, n_2}(q)$ ($n_1, n_2 \geq 1$) do not satisfy the shuffle product formulas.

In general, we define $h(x_1, \dots, x_r)$ as an image of the monomial $\left(\begin{smallmatrix} 1, \dots, 1 \\ x_1, \dots, x_r \end{smallmatrix}\right)$ under the algebra homomorphism $H \circ \exp$, which is given by

$$h(x_1, \dots, x_r) = \sum_{(i_1, i_2, \dots, i_m)} \frac{1}{i_1! i_2! \cdots i_m!} H\left(\begin{smallmatrix} i_1, i_2, \dots, i_m \\ x'_{i_1}, x'_{i_2}, \dots, x'_{i_m} \end{smallmatrix}\right), \quad (4.2)$$

where the sum runs over all decompositions of the integer r as a sum of positive integers and the variables are given by $x'_{i_1} = x_1 + \cdots + x_{i_1}$, $x'_{i_2} = x_{i_1+1} + \cdots + x_{i_1+i_2}$, \dots , $x'_{i_m} = x_{i_1+\cdots+i_{m-1}+1} + \cdots + x_r$. It follows that the power series $h(x_1, \dots, x_r)$ satisfies the shuffle relation below.

$$h(x_1, \dots, x_r)h(x_{r+1}, \dots, x_{r+s}) = h(x_1, \dots, x_{r+s})|sh_r^{(r+s)}, \quad (4.3)$$

where $sh_r^{(r+s)} = \sum_{\sigma \in \Sigma(r, s)} \sigma$ in the group ring $\mathbb{Z}[\mathfrak{S}_{r+s}]$ (for the set $\Sigma(r, s)$, see (I2)), and the symmetric group \mathfrak{S}_r acts on $\mathcal{K}[[x_1, \dots, x_r]]$ in the obvious way by $(f|\sigma)(x_1, \dots, x_r) = f(x_{\sigma^{-1}(1)}, \dots, x_{\sigma^{-1}(r)})$ (it defines a right action, i.e. $f|(\sigma\tau) = (f|\sigma)|\tau$) with extending to the group ring $\mathbb{Z}[\mathfrak{S}_r]$ by linearity. As in the case of $r = 2$, we set

$$g_{\text{m}}(x_1, \dots, x_r) := h(x_r - x_{r-1}, \dots, x_2 - x_1, x_1). \quad (4.4)$$

With the coefficients of (4.4), we define a \mathbb{Q} -linear map $\mathfrak{g}^{\mathfrak{m}} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{C}[[q]]$ and prove that the map $\mathfrak{g}^{\mathfrak{m}}$ is an algebra homomorphism.

Definition 4.3. We define the \mathbb{Q} -linear map $\mathfrak{g}^{\mathfrak{m}} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{C}[[q]]$ by

$$\mathfrak{g}^{\mathfrak{m}}(I(n_1, \dots, n_r)) = g_{n_1, \dots, n_r}^{\mathfrak{m}}(q)$$

and $\mathfrak{g}^{\mathfrak{m}}(1) = 1$, where the q -series $g_{n_1, \dots, n_r}^{\mathfrak{m}}(q)$ is given by the coefficient of $x_1^{n_1-1} \dots x_r^{n_r-1}$ in

$$g_{\mathfrak{m}}(-2\pi\sqrt{-1}x_1, \dots, -2\pi\sqrt{-1}x_r) = \sum_{n_1, \dots, n_r > 0} g_{n_1, \dots, n_r}^{\mathfrak{m}}(q) x_1^{n_1-1} \dots x_r^{n_r-1}.$$

Theorem 4.4. The map $\mathfrak{g}^{\mathfrak{m}} : \mathcal{I}_{\bullet}^1 \rightarrow \mathbb{C}[[q]]$ is an algebra homomorphism.

Proof. It is sufficient to show that for any integers $r, s \geq 1$ the generating function $g_{\mathfrak{m}}(x_1, \dots, x_{r+s})$ satisfies the shuffle relation:

$$g_{\mathfrak{m}}^{\sharp}(x_1, \dots, x_r) g_{\mathfrak{m}}^{\sharp}(x_{r+1}, \dots, x_{r+s}) = g_{\mathfrak{m}}^{\sharp}(x_1, \dots, x_{r+s}) \Big| sh_r^{(r+s)}, \quad (4.5)$$

where the operator \sharp is the change of variables defined by $f^{\sharp}(x_1, \dots, x_r) = f(x_1, x_1 + x_2, \dots, x_1 + \dots + x_r)$ (remark that this expression of the shuffle relation is also found in [10, Proof of Proposition 7] with the opposite convention). For integers $r, s \geq 1$, let

$$\rho_{r,s} = \begin{pmatrix} 1 & 2 & \dots & r & r+1 & \dots & r+s-1 & r+s \\ r & r-1 & \dots & 1 & r+s & \dots & r+2 & r+1 \end{pmatrix} \in \mathfrak{S}_{r+s}.$$

Applying the operator \sharp to both sides of (4.4) we obtain $g_{\mathfrak{m}}^{\sharp}(x_1, \dots, x_r) = h(x_r, \dots, x_1)$ and therefore by (4.3) the left-hand side of (4.5) is reduced to

$$\begin{aligned} (\text{LHS}) &= h(x_r, \dots, x_1) h(x_{r+s}, \dots, x_{r+1}) \\ &= h(x_1, \dots, x_r) h(x_{r+1}, \dots, x_{r+s}) \Big| \rho_{r,s} \\ &= h(x_1, \dots, x_{r+s}) \Big| sh_r^{(r+s)} \Big| \rho_{r,s} \\ &= g_{\mathfrak{m}}^{\sharp}(x_1, \dots, x_{r+s}) \Big| \tau_{r+s} \Big| sh_r^{(r+s)} \Big| \rho_{r,s}, \end{aligned}$$

where we set $\tau_r = \begin{pmatrix} 1 & 2 & \cdots & r \\ r & r-1 & \cdots & 1 \end{pmatrix} \in \mathfrak{S}_r$. For any $\sigma \in \Sigma(r, s)$ (recall (I2)), one easily finds $\tau_{r+s}\sigma\rho_{r,s} \in \Sigma(r, s)$, and hence

$$g_{\text{III}}^\sharp(x_1, \dots, x_{r+s}) | \tau_{r+s} | sh_r^{(r+s)} | \rho_{r,s} = g_{\text{III}}^\sharp(x_1, \dots, x_{r+s}) | sh_r^{(r+s)},$$

which completes the proof. \square

4.2 The double shuffle relation for regularised multiple Eisenstein series

In this subsection, we prove the double shuffle relations for regularised multiple Eisenstein series (Theorem 1.2).

The regularised multiple Eisenstein series $G_{n_1, \dots, n_r}^{\text{III}}(q)$ is defined as follows.

Definition 4.5. For integers $n_1, \dots, n_r \geq 1$ we define the q -series $G_{n_1, \dots, n_r}^{\text{III}}(q)$ by

$$G_{n_1, \dots, n_r}^{\text{III}}(q) = (\mathfrak{z}^{\text{III}} \otimes \mathfrak{g}^{\text{III}}) \circ \Delta(I(n_1, \dots, n_r)).$$

We remark that one can easily deduce that our $G_{n_1, n_2}^{\text{III}}(q)$ coincides with Kaneko's double Eisenstein series [11].

We begin by showing a connection with the multiple Eisenstein series $G_{n_1, \dots, n_r}(\tau)$, which can be regarded as an analogue of (3.2).

Theorem 4.6. For integers $n_1, \dots, n_r \geq 2$, with $q = e^{2\pi\sqrt{-1}\tau}$ we have

$$G_{n_1, \dots, n_r}^{\text{III}}(q) = G_{n_1, \dots, n_r}(\tau).$$

Proof. As in the proof of Theorem 1.1, it suffices to show that for each word $w_1 \cdots w_r$ of length r in $\{\mathbf{x}, \mathbf{y}\}^*$ and integers $n_1, \dots, n_r \geq 2$, we have

$$(\mathfrak{z}^{\text{III}} \otimes \mathfrak{g}^{\text{III}})(\psi_{n_1, \dots, n_r}(w_1 \cdots w_r)) = G_{n_1, \dots, n_r}(w_1 \cdots w_r).$$

This immediately follows from the next identity: for integers $n_1, \dots, n_r \geq 2$

$$g_{n_1, \dots, n_r}^{\text{III}}(q) = g_{n_1, \dots, n_r}(q).$$

Combining (4.4) with (4.2), we have

$$g_{\mathfrak{m}}(x_1, \dots, x_r) = \sum_{(i_1, i_2, \dots, i_m)} \frac{1}{i_1! i_2! \cdots i_m!} H\left(\begin{matrix} i_1, i_2, \dots, i_m \\ x''_{i_1}, x''_{i_2}, \dots, x''_{i_m} \end{matrix}\right),$$

where (i_1, \dots, i_m) runs over all decompositions of the integer r as a sum of positive integers and $x''_{i_1} = x_r - x_{r-i_1}$, $x''_{i_2} = x_{r-i_1} - x_{r-i_1-i_2}$, \dots , $x''_{i_m} = x_{r-i_1-\dots-i_{m-1}}$. When $m < r$ (i.e. $i_j > 1$ for some $j \in \{1, 2, \dots, m\}$), there is no contribution to $g_{n_1, \dots, n_r}^{\mathfrak{m}}(q)$ with $n_1, \dots, n_r \geq 2$ from the coefficients of the power series $H\left(\begin{matrix} i_1, i_2, \dots, i_m \\ x''_{i_1}, x''_{i_2}, \dots, x''_{i_m} \end{matrix}\right)$ because it lies in $\mathcal{K}[[x_r, x_{r-i_1}, \dots, x_{r-i_1-\dots-i_{m-1}}]]$. Thus the contribution to $g_{n_1, \dots, n_r}^{\mathfrak{m}}(q)$ with $n_1, \dots, n_r \geq 2$ is only the coefficient of $x_1^{n_1-1} \cdots x_r^{n_r-1} / (-2\pi\sqrt{-1})^{n_1+\dots+n_r}$ in $H\left(\begin{matrix} 1, \dots, 1, 1 \\ x_r - x_{r-1}, \dots, x_2 - x_1, x_1 \end{matrix}\right)$, which by Proposition 4.1 is $g_{n_1, \dots, n_r}(q)$. This completes the proof. \square

Let us give the precise statement of Theorem 1.2. The harmonic product $*$ on \mathfrak{H}^1 is defined inductively by

$$y_{n_1} w * y_{n_2} w' = y_{n_1} (w * y_{n_2} w') + y_{n_2} (y_{n_1} w * w') + y_{n_1+n_2} (w * w'),$$

and $w * 1 = 1 * w = w$ for $y_{n_1}, y_{n_2} \in \mathfrak{H}^1$ and words w, w' in \mathfrak{H}^1 , together with \mathbb{Q} -bilinearity. For each word $w \in \mathfrak{H}^1$, the dual element of w is denoted by $c_w \in (\mathfrak{H}^1)^\vee = \text{Hom}(\mathfrak{H}^1, \mathbb{Q})$ such that $c_w(v)$ is 1 if $w = v$ and 0 otherwise. If w is the empty word \emptyset , c_w kills $\mathfrak{H}_{>0}^1$ and $c_w(1) = 1$. With this we define the \mathbb{Q} -bilinear map $\text{har} : \mathcal{I}_\bullet^1 \times \mathcal{I}_\bullet^1 \rightarrow \mathcal{I}_\bullet^1$ by

$$\text{har}(I(w_1), I(w_2)) = \sum_{w \in \{y_1, y_2, y_3, \dots\}^*} c_w(w_1 * w_2) I(w)$$

for words $w_1, w_2 \in \mathfrak{H}^1$, where we identify $I(w) = I(n_1, \dots, n_r)$ for $w = y_{n_1} \cdots y_{n_r}$.

Theorem 4.7. *For any words w_1, w_2 in $\{y_2, y_3, y_4, \dots\}^*$, one has*

$$(\mathfrak{z}^{\mathfrak{m}} \otimes \mathfrak{g}^{\mathfrak{m}}) \circ \Delta(\text{har}(I(w_1), I(w_2)) - I(w_1)I(w_2)) = 0.$$

Proof. Consider the following holomorphic function on the upper half-plane:

for integers L, M

$$G_{n_1, \dots, n_r}^{(L, M)}(\tau) = \sum_{\substack{0 < \lambda_1 < \dots < \lambda_r \\ \lambda_i \in \mathbb{Z}_L \tau + \mathbb{Z}_M}} \frac{1}{\lambda_1^{n_1} \dots \lambda_r^{n_r}}.$$

Write $G_w^{(L, M)}(\tau) = G_{n_1, \dots, n_r}^{(L, M)}(\tau)$ for each word $w = y_{n_1} \dots y_{n_r}$. By definition, it follows that these functions satisfy the harmonic product: for any words $w_1, w_2 \in \mathfrak{H}^1$, one has

$$G_{w_1}^{(L, M)}(\tau) G_{w_2}^{(L, M)}(\tau) = \sum_{w \in \{y_1, y_2, y_3, \dots\}^*} c_w(w_1 * w_2) G_w^{(L, M)}(\tau). \quad (4.6)$$

Since the harmonic product $*$ preserves the space $\mathfrak{H}^2 := \mathbb{Q}\langle y_2, y_3, y_4, \dots \rangle$, taking $\lim_{L \rightarrow \infty} \lim_{M \rightarrow \infty}$ for both sides of (4.6), one has for words $w_1, w_2 \in \mathfrak{H}^2$

$$G_{w_1}(\tau) G_{w_2}(\tau) = \sum_{w \in \{y_2, y_3, y_4, \dots\}^*} c_w(w_1 * w_2) G_w(\tau).$$

Then the result follows from Theorem 4.6 and the fact that the map $(\mathfrak{z}^{\text{m}} \otimes \mathfrak{g}^{\text{m}}) \circ \Delta : \mathcal{I}_\bullet^1 \rightarrow \mathbb{C}[[q]]$ is an algebra homomorphism (Propositions 3.4, 3.6 and Theorem 4.4). \square

The first example of \mathbb{Q} -linear relations among G^{m} 's is

$$G_4^{\text{m}}(q) - 4G_{1,3}^{\text{m}}(q) = 0, \quad (4.7)$$

which comes from $\text{har}(I(2), I(2)) - I(2)^2$. The following is the table of the number of linearly independent relations provided by Theorem 4.7 (we will see that Theorem 4.7 is not enough to capture all relations when $N \geq 5$).

N	0	1	2	3	4	5	6	7	8	9	10
$\#rel.$	0	0	0	0	1	1	3	5	11	19	37

4.3 Further problems

We end this paper by mentioning the dimension of the space of G^{m} 's. For convenience, we use a normalisation for all objects: for a sequence $\{\gamma_{n_1, \dots, n_r}\}$ in-

dexed by positive integers n_1, \dots, n_r , write $\tilde{\gamma}_{n_1, \dots, n_r} = \gamma_{n_1, \dots, n_r} / (-2\pi\sqrt{-1})^{n_1 + \dots + n_r}$. As usual, we call $n_1 + \dots + n_r$ the weight and γ_{n_1, \dots, n_r} admissible if $n_r \geq 2$. Let \mathcal{E}_N (resp. $\mathcal{Q}^{(N)}$) be the \mathbb{Q} -vector space spanned by all admissible \tilde{G}^{m} 's (resp. \tilde{g}^{m} 's) of weight N (resp. less than or equal to N). Set $\mathcal{E}_0 = \mathcal{Q}^{(0)} = \mathbb{Q}$. It is not difficult to deduce that each \mathbb{Q} -linear relation among \tilde{G}^{m} 's of the form $\sum a_w \tilde{G}_w^{\text{m}}(q) = 0$ ($a_w \in \mathbb{Q}$) gives rise to a \mathbb{Q} -linear relation among \tilde{g}^{m} 's modulo lower weight of the form $\sum a_w \tilde{g}_w^{\text{m}}(q) \equiv 0 \pmod{\mathcal{Q}^{(N-1)}}$, where the both sums run over admissible indices of weight N . For instance, the relation (4.7) provides the relation $-\frac{1}{6}\tilde{g}_2^{\text{m}}(q) + \tilde{g}_4^{\text{m}}(q) - 4\tilde{g}_{1,3}^{\text{m}}(q) = 0$, where we actually have used the known relations $\tilde{\zeta}(2) = -1/24$ and $\tilde{\zeta}(1, 3) = \tilde{\zeta}(4) = 1/1440$. Thus we obtain the surjective map, which is an algebra homomorphism, from the graded \mathbb{Q} -algebra $\mathcal{E} := \bigoplus_{N \geq 0} \mathcal{E}_N$ (taking the formal direct sum) to the graded \mathbb{Q} -algebra $\bigoplus_{N \geq 0} \mathcal{Q}^{(N)} / \mathcal{Q}^{(N-1)}$ given by $\tilde{G}_{n_1, \dots, n_r}^{\text{m}}(q) \mapsto \tilde{g}_{n_1, \dots, n_r}^{\text{m}}(q) \pmod{\mathcal{Q}^{(N-1)}}$. From this, we have

$$\dim_{\mathbb{Q}} \mathcal{Q}^{(N)} / \mathcal{Q}^{(N-1)} \leq \dim_{\mathbb{Q}} \mathcal{E}_N.$$

The second author performed numerical experiments of the dimension of the above vector spaces up to $N = 7$. The list of (upper bounds of) the dimension is given as follows.

N	2	3	4	5	6	7
$\dim_{\mathbb{Q}} \mathcal{E}_N$	1	2	3	≤ 6	≤ 10	≤ 18
$\dim_{\mathbb{Q}} \mathcal{Q}^{(N)} / \mathcal{Q}^{(N-1)}$	1	2	3	6	10	18

Interestingly, the above sequences coincide with the table [2, Table 5] (up to $N = 7$) which is the list of the dimension of the space spanned by all admissible \tilde{g} 's modulo lower weight (they denote $\tilde{g}_{n_1, \dots, n_r}(q)$ by $[n_r, \dots, n_1]$ and indicate that the above sequence is given by the sequence $\{d'_N\}_{N \geq 2}$ defined by $d'_N = 2d'_{N-2} + 2d'_{N-3}$ for $N \geq 5$ with the initial values $d'_2 = 1, d'_3 = 2, d'_4 = 3$). It is also interesting to note that the \mathbb{Q} -algebra \mathcal{E} contains the ring $\mathbb{Q}[\tilde{G}_2^{\text{m}}, \tilde{G}_4^{\text{m}}, \tilde{G}_6^{\text{m}}]$ of quasimodular forms for $\text{SL}_2(\mathbb{Z})$ over \mathbb{Q} , which is closed under the derivative $d = qd/dq$ (see [13]). It would be very interesting to consider whether the \mathbb{Q} -algebra \mathcal{E} is closed under the derivative, because by expressing $d\tilde{G}^{\text{m}}$ as \mathbb{Q} -linear combinations of \tilde{G}^{m} 's and taking the constant term as an element in $\mathbb{C}[[q]]$ one obtains \mathbb{Q} -linear relations among multiple

zeta values. For this, one can show that for $N \geq 1$ we have

$$d\tilde{G}_N^m(q) = 2N(\tilde{G}_{N+2}^m(q) - \sum_{i=1}^N \tilde{G}_{i,N+2-i}^m(q)),$$

which was first proved by Kaneko [11]. We hope to discuss these problems in a future publication.

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Appendix C

The algebra of bi-brackets and regularized multiple Eisenstein series

The algebra of bi-brackets and regularized multiple Eisenstein series

HENRIK BACHMANN

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Abstract

We study the algebra of certain q -series, called bi-brackets, whose coefficients are given by weighted sums over partitions. These series incorporate the theory of modular forms for the full modular group as well as the theory of multiple zeta values (MZV) due to their appearance in the Fourier expansion of regularized multiple Eisenstein series. Using the conjugation of partitions we obtain linear relations between bi-brackets, called the partition relations, which yield naturally two different ways of expressing the product of two bi-brackets similar to the stuffle and shuffle product of multiple zeta values. Bi-brackets are generalizations of the generating functions of multiple divisor sums, called brackets, $[s_1, \dots, s_l]$ studied in [BK]. We use the algebraic structure of bi-brackets to define further q -series $[s_1, \dots, s_l]^{\sqcup}$ and $[s_1, \dots, s_l]^*$ which satisfy the shuffle and stuffle product formulas of MZV by using results about quasi-shuffle algebras introduced by Hoffman. In [BT] regularized multiple Eisenstein series G^{\sqcup} were defined, by using an explicit connection to the coproduct on formal iterated integrals. These satisfy the shuffle product formula. Applying the same concept for the coproduct on quasi-shuffle algebras enables us to define multiple Eisenstein series G^* satisfying the stuffle product. We show that both G^{\sqcup} and G^* are given by linear combinations of products of MZV and bi-brackets. Comparing these two regularized multiple Eisenstein series enables us to obtain finite double shuffle relations for multiple Eisenstein series in low weights which extend the relations proven in [BT].

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1 Introduction

Multiple zeta values are natural generalizations of the Riemann zeta values that are defined for integers $s_1 > 1$ and $s_i \geq 1$ for $i > 1$ by

$$\zeta(s_1, \dots, s_l) := \sum_{n_1 > n_2 > \dots > n_l > 0} \frac{1}{n_1^{s_1} \dots n_l^{s_l}}.$$

Because of its occurrence in various fields of mathematics and physics these real numbers are of particular interest. The \mathbb{Q} -vector space of all multiple zeta values of weight k is then given by

$$\mathcal{MZ}_k := \langle \zeta(s_1, \dots, s_l) \mid s_1 + \dots + s_l = k \text{ and } l > 0 \rangle_{\mathbb{Q}}.$$

It is well known that the product of two multiple zeta values can be written as a linear combination of multiple zeta values of the same weight by using the stuffle or shuffle relations. Thus they generate a \mathbb{Q} -algebra \mathcal{MZ} . There are several connections of these numbers to modular forms for the full modular group. Some of them are treated in [GKZ], where connections of double zeta values and modular forms are described. One of them is given by double Eisenstein series $G_{s_1, s_2} \in \mathbb{C}[[q]]$ which are the length two version of classical Eisenstein series and which are given by a double sum over ordered lattice points. These functions have a Fourier expansion given by sums of products of MZV and certain q -series with the double zeta value $\zeta(s_1, s_2)$ as their constant term. In [Ba] the author treated the multiple case and calculated the Fourier expansion of multiple Eisenstein series (MES) $G_{s_1, \dots, s_l} \in \mathbb{C}[[q]]$. The result of [Ba] was that the Fourier expansion of MES is again a linear combination of MZV and q -series $[s_1, \dots, s_l] \in \mathbb{Q}[[q]]$, called brackets, with the corresponding MZV as the constant term. For example it is

$$\begin{aligned} G_{3,2,2}(\tau) = & \zeta(3, 2, 2) + \left(\frac{54}{5} \zeta(2, 3) + \frac{51}{5} \zeta(3, 2) \right) (2\pi i)^2 [2] + \frac{16}{3} \zeta(2, 2) (2\pi i)^3 [3] \\ & + 3\zeta(3) (2\pi i)^4 [2, 2] + 4\zeta(2) (2\pi i)^5 [3, 2] + (2\pi i)^7 [3, 2, 2]. \end{aligned}$$

It turned out that the q -series $[s_1, \dots, s_l]$, whose coefficients a_n are given by weighted sums over partitions of n , are, independently to their appearance in the Fourier expansion of MES, very interesting objects and therefore they were studied on their own in

[BK]. There the authors studied the algebraic structure of the space \mathcal{MD} spanned by these brackets and we will refine, generalize and use some of the results in this note.

Due to convergence issues the MES are just defined for $s_1, \dots, s_l \geq 2$ and therefore there are a lot more MZV than MES. A natural question was therefore the following

Question 1. *What is a "good" definition of a "regularized" multiple Eisenstein series, such that for each multiple zeta value $\zeta(s_1, \dots, s_l)$ with $s_1 > 1, s_2, \dots, s_l \geq 1$ there is a multiple Eisenstein series*

$$G_{s_1, \dots, s_l}^{reg} = \zeta(s_1, \dots, s_l) + \sum_{n>0} a_n q^n \in \mathbb{C}[[q]]$$

with this multiple zeta values as the constant term in its Fourier expansion and which equals the original multiple Eisenstein series in the case $s_1, \dots, s_l \geq 2$?

By "good" we mean that these multiple Eisenstein series should have the same, or at least as much as possible, algebraic structure as multiple zeta values, i.e. they should fulfill the shuffle or/and the stuffle product. In [BT] the authors addressed this question and they define (shuffle) regularized MES $G_{s_1, \dots, s_l}^{\sqcup}$, defined for all $s_1, \dots, s_l \in \mathbb{N}$, which coincide with the G_{s_1, \dots, s_l} in the case $s_1, \dots, s_l \geq 2$ and which fulfill the shuffle product. In their construction the authors consider certain q -series similar to the brackets which also fulfill the shuffle product.

In this note we want to consider a more general class of q -series which we call bi-brackets. We will see that the q -series appearing in the construction in [BT] are linear combination of bi-brackets. Furthermore we will address the above question with respect to the stuffle product and we will construct another (stuffle) regularized type of MES, denoted by G_{s_1, \dots, s_l}^* , satisfying the stuffle product formula. The bi-brackets will also appear there and we will be able to write G^{\sqcup} and G^* as sums of products of MZV and bi-brackets which then enables us to compare these two types of regularized MES.

Even when one is not interested in the question of extending the definition of MES we want to emphasize the reader that these q -series are interesting by their own rights, since they give a q -analogue of multiple zeta values with a nice algebraic structure. These q -analogues have two ways to write the product of two such series similar to the shuffle and the stuffle product for MZV. For $s_1, \dots, s_l \geq 1, r_1, \dots, r_l \geq 0$ these q -series, which we call bi-brackets, are given by

$$\left[\begin{matrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{matrix} \right] := \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \frac{u_1^{r_1}}{r_1!} \dots \frac{u_l^{r_l}}{r_l!} \cdot \frac{v_1^{s_1-1} \dots v_l^{s_l-1}}{(s_1-1)! \dots (s_l-1)!} \cdot q^{u_1 v_1 + \dots + u_l v_l} \in \mathbb{Q}[[q]].$$

In the first section we will interpret this sum as a weighted sum over partitions of a natural number n . The conjugation of partitions will give us linear relations between the bi-brackets which we therefore call the partition relation. We use this relation to prove a stuffle and shuffle analogue of the product of two bi-brackets and obtain for

example

$$\begin{bmatrix} 2, 3 \\ 0, 0 \end{bmatrix} + \begin{bmatrix} 3, 2 \\ 0, 0 \end{bmatrix} + \begin{bmatrix} 5 \\ 0 \end{bmatrix} - \frac{1}{12} \begin{bmatrix} 3 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 3 \\ 0 \end{bmatrix} = \begin{bmatrix} 2, 3 \\ 0, 0 \end{bmatrix} + 3 \begin{bmatrix} 3, 2 \\ 0, 0 \end{bmatrix} + 6 \begin{bmatrix} 4, 1 \\ 0, 0 \end{bmatrix} - 3 \begin{bmatrix} 4 \\ 0 \end{bmatrix} + 3 \begin{bmatrix} 4 \\ 1 \end{bmatrix}.$$

Compare this with the "real" stuffle and shuffle product of multiple zeta values

$$\zeta(2, 3) + \zeta(3, 2) + \zeta(5) = \zeta(2) \cdot \zeta(3) = \zeta(2, 3) + 3\zeta(3, 2) + 6\zeta(4, 1).$$

Using the algebraic structure of the space of bi-brackets we define a shuffle $[s_1, \dots, s_l]^\sqcup$ and stuffle $[s_1, \dots, s_l]^*$ version of the ordinary brackets as certain linear combination of bi-brackets. These objects fulfill the same shuffle and stuffle products as multiple zeta values. Both constructions use the theory of quasi-shuffle algebras developed by Hoffman in [H]. We end the introduction by summarizing the results of this paper on bi-brackets and regularized multiple Eisenstein series in the following two vaguely formulated theorems:

Theorem A. i) The space \mathcal{BD} spanned by all bi-brackets ${}_{r_1, \dots, r_l}^{s_1, \dots, s_l}$ forms a \mathbb{Q} -algebra with the space of (quasi-)modular forms and the space \mathcal{MD} of brackets as subalgebras. There are two ways to express the product as a linear combination of bi-brackets which yields a large family of linear relations.

ii) There are two subalgebras $\mathcal{MD}^\sqcup \subset \mathcal{BD}$ and $\mathcal{MD}^* \subset \mathcal{MD}$ spanned by elements $[s_1, \dots, s_l]^\sqcup$ and $[s_1, \dots, s_l]^*$ which fulfill the shuffle and stuffle products, respectively, and which are in the length one case given by the bracket $[s_1]$.

For example we have similarly to the relation between MZV above

$$[2, 3]^* + [3, 2]^* + [5] = [2] \cdot [3] = [2, 3]^\sqcup + 3[3, 2]^\sqcup + 6[4, 1]^\sqcup.$$

Denote by $\mathcal{MZB} \subset \mathbb{C}[[q]]$ the space of all formal power series in q which can be written as a linear combination of products of MZV, powers of $(-2\pi i)$ and bi-brackets.

Theorem B. i) The shuffle regularized multiple Eisenstein series $G_{s_1, \dots, s_l}^\sqcup \in \mathbb{C}[[q]]$ defined in [BT] can be written as a linear combination of products of MZV, powers of $(-2\pi i)$ and shuffle brackets $[r_1, \dots, r_m]^\sqcup$, i.e. they are elements of the space \mathcal{MZB} .

ii) For all $s_1, \dots, s_l \in \mathbb{N}$ and $M \in \mathbb{N}$ there are q -series $G_{s_1, \dots, s_l}^{*, M} \in \mathbb{C}[[q]]$ (see Definition 6.12) which fulfill the stuffle product. If the limit $G_{s_1, \dots, s_l}^* := \lim_{M \rightarrow \infty} G_{s_1, \dots, s_l}^{*, M}$ exists it will be an element in \mathcal{MZB} which still fulfills the stuffle product. In that case the q -series G_{s_1, \dots, s_l}^* will be called stuffle regularized multiple Eisenstein series.

iii) For $s_1, \dots, s_l \geq 2$ both regularized multiple Eisenstein series equal the classical multiple Eisenstein series, i.e. we have

$$G_{s_1, \dots, s_l} = G_{s_1, \dots, s_l}^\sqcup = G_{s_1, \dots, s_l}^*.$$

Content of this paper: In section 2 we will introduce bi-brackets and their generating series. We will show that there are a natural linear relations between bi-brackets, called the partition relations. In section 3 we prove that the algebra of bi-brackets has the structure of a quasi-shuffle algebra in the sense of [H]. The partition relation will yield another way of multiplying two bi-brackets which differs from the quasi-shuffle product and which therefore yields linear relations similar to the double shuffle relations of MZV. The connection to modular forms and the derivatives of bi-brackets will be subject of section 4. We will see that relations between bi-brackets can be used to prove relations between modular forms and vice versa. Section 5 will be devoted to the definition of the brackets $[s_1, \dots, s_l]^{\sqcup}$ and $[s_1, \dots, s_l]^*$. For this we will recall the algebraic setup of Hoffman in this section. Finally in section 4 we will recall the results of [BT] and the definition of the shuffle regularized MES G^{\sqcup} . After this we will define the stuffle regularized MES $G^{*,M}$ and G^* by using a similar approach as in the definition of G^{\sqcup} . We end section 4 by comparing these two regularized MES in low weights.

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2 Bi-brackets and their generating series

As motivated in the introduction we want to study the following q -series:

Definition 2.1. For $r_1, \dots, r_l \geq 0$, $s_1, \dots, s_l > 0$ and we define the following q -series

$$\left[\begin{matrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{matrix} \right] := \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \frac{u_1^{r_1}}{r_1!} \cdots \frac{u_l^{r_l}}{r_l!} \cdot \frac{v_1^{s_1-1} \cdots v_l^{s_l-1}}{(s_1-1)! \cdots (s_l-1)!} \cdot q^{u_1 v_1 + \dots + u_l v_l} \in \mathbb{Q}[[q]]$$

which we call *bi-brackets* of weight $r_1 + \dots + r_l + s_1 + \dots + s_l$, upper weight $s_1 + \dots + s_l$, lower weight $r_1 + \dots + r_l$ and length l . By \mathcal{BD} we denote the \mathbb{Q} -vector space spanned by all bi-brackets and 1.

The factorial factors in the definition will become clear when considering their generating functions and the connection to multiple zeta values. For $r_1 = \dots = r_l = 0$

the bi-brackets are just the brackets

$$\begin{bmatrix} s_1, \dots, s_l \\ 0, \dots, 0 \end{bmatrix} = [s_1, \dots, s_l]$$

as defined and studied in [BK]. The space spanned by all brackets form a differential \mathbb{Q} -algebra \mathcal{MD} with the differential given by $d_q = q \frac{d}{dq}$. We will see that the bi-brackets are also closed under the multiplication of formal power series and therefore \mathcal{BD} is a \mathbb{Q} -algebra with subalgebra \mathcal{MD} (see Theorem 3.6).

Definition 2.2. For the generating function of the bi-brackets we write

$$\begin{vmatrix} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{vmatrix} := \sum_{\substack{s_1, \dots, s_l > 0 \\ r_1, \dots, r_l > 0}} \begin{bmatrix} s_1, \dots, s_l \\ r_1 - 1, \dots, r_l - 1 \end{bmatrix} X_1^{s_1-1} \dots X_l^{s_l-1} \cdot Y_1^{r_1-1} \dots Y_l^{r_l-1}.$$

These are elements in the ring $\mathcal{BD}_{\text{gen}} = \varinjlim_j \mathcal{BD}[[X_1, \dots, X_j, Y_1, \dots, Y_j]]$ of all generating series of bi-brackets.

To derive relations between bi-brackets we will prove functional equations for their generating functions. The key fact for this is that there are two different ways of expressing these given by the following Theorem.

Theorem 2.3. For $n \in \mathbb{N}$ set

$$E_n(X) := e^{nX} \quad \text{and} \quad L_n(X) := \frac{e^X q^n}{1 - e^X q^n} \in \mathbb{Q}[[q, X]].$$

Then for all $l \geq 1$ we have the following two different expressions for the generating functions:

$$\begin{aligned} \begin{vmatrix} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{vmatrix} &= \sum_{u_1 > \dots > u_l > 0} \prod_{j=1}^l E_{u_j}(Y_j) L_{u_j}(X_j) \\ &= \sum_{u_1 > \dots > u_l > 0} \prod_{j=1}^l E_{u_j}(X_{l+1-j} - X_{l+2-j}) L_{u_j}(Y_1 + \dots + Y_{l-j+1}) \end{aligned}$$

(with $X_{l+1} := 0$). In particular the *partition relations* holds:

$$\begin{vmatrix} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{vmatrix} \stackrel{P}{=} \begin{vmatrix} Y_1 + \dots + Y_l, \dots, Y_1 + Y_2, Y_1 \\ X_l, X_{l-1} - X_l, \dots, X_1 - X_2 \end{vmatrix}. \quad (2.1)$$

Proof. First rewrite the generating function as

$$\begin{aligned} \begin{vmatrix} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{vmatrix} &= \sum_{\substack{s_1, \dots, s_l > 0 \\ r_1, \dots, r_l > 0 \\ u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \prod_{j=1}^l \frac{u_j^{r_j-1}}{(r_j-1)!} \frac{v_j^{s_j-1}}{(s_j-1)!} q^{u_j v_j} X_j^{s_j-1} Y_j^{r_j-1} \\ &= \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \prod_{j=1}^l e^{v_j X_j} e^{u_j Y_j} q^{u_j v_j} \end{aligned}$$

The first statement follows directly by using the geometric series because

$$\sum_{v>0} e^{vX} q^{uv} = \frac{e^X q^u}{1 - e^X q^u} = L_u(X)$$

For the second statement set $u_j = u'_1 + \dots + u'_{l-j+1}$ and $v'_j = v_1 + \dots + v_{l-j+1}$ (i.e. $v_j = v'_{l-j+1} - v'_{l-j+2}$ and $v_{l+1} := 0$) for $1 \leq j \leq l$. This gives

$$\begin{aligned} q^{u_1 v_1 + \dots + u_l v_l} &= q^{(u'_1 + \dots + u'_l) v_1 + (u'_1 + \dots + u'_{l-1}) v_2 + \dots + u'_1 v_l} \\ &= q^{(v_1 + \dots + v_l) u'_1 + \dots + v_1 u'_l} = q^{v'_1 u'_1 + \dots + v'_l u'_l} \end{aligned}$$

and the summation over $u_1 > \dots > u_l > 0$ and $v_1, \dots, v_l > 0$ changes to a summation over $u'_1, \dots, u'_l > 0$ and $v'_1 > \dots > v'_l > 0$ and therefore we obtain

$$\begin{aligned} \sum_{\substack{u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} \prod_{j=1}^l e^{v_j X_j} e^{u_j Y_j} q^{u_j v_j} &= \sum_{\substack{v'_1 > \dots > v'_l > 0 \\ u'_1, \dots, u'_l > 0}} \prod_{j=1}^l e^{(v'_{l-j+1} - v'_{l-j+2}) X_j} e^{(u'_1 + \dots + u'_{l-j+1}) Y_j} q^{v'_j u'_j} \\ &= \sum_{v'_1 > \dots > v'_l > 0} \prod_{j=1}^l e^{v'_j (X_{l-j+1} - X_{l-j+2})} L_{v'_j} (Y_1 + \dots + Y_{l-j+1}) \end{aligned}$$

which is exactly the representation of the generating function. \square

Compare the relation (2.1) to the conjugation (2.2) of partitions given at the end of this section.

Remark 2.4. i) The bi-brackets and their generating series also give examples of what is called a bimould by Ecalle in [E]. In his language the equation (2.1) states that the bimould of generating series of bi-brackets is swap invariant.

ii) In [Zu] the author studied a variation of the bi-brackets, namely the series

$$\mathfrak{Z} \left[\begin{matrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{matrix} \right] = \sum_{\substack{m_1, \dots, m_l > 0 \\ d_1, \dots, d_l > 0}} \frac{m_1^{r_1-1} d_1^{s_1-1} \dots m_l^{r_l-1} d_l^{s_l-1} q^{(m_1 + \dots + m_l) d_1 + \dots + m_l d_l}}{(r_1 - 1)! (s_1 - 1)! \dots (r_l - 1)! (s_l - 1)!},$$

which he calls multiple q -zeta brackets. These can be written in terms of bi-brackets and vice versa. For this model the equation (2.1), which in [Zu] is called duality, has the nice form

$$\mathfrak{Z} \left[\begin{matrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{matrix} \right] = \mathfrak{Z} \left[\begin{matrix} s_l, \dots, s_1 \\ r_l, \dots, r_1 \end{matrix} \right].$$

Corollary 2.5. (Partition relation in length one and two) For $r, r_1, r_2 \geq 0$ and $s, s_1, s_2 > 0$ we have the following relations in length one and two

$$\begin{aligned} \begin{bmatrix} s \\ r \end{bmatrix} &= \begin{bmatrix} r+1 \\ s-1 \end{bmatrix}, \\ \begin{bmatrix} s_1, s_2 \\ r_1, r_2 \end{bmatrix} &= \sum_{\substack{0 \leq j \leq r_1 \\ 0 \leq k \leq s_2-1}} (-1)^k \binom{s_1-1+k}{k} \binom{r_2+j}{j} \begin{bmatrix} r_2+j+1, r_1-j+1 \\ s_2-1-k, s_1-1+k \end{bmatrix}. \end{aligned}$$

Proof. In the smallest cases the Theorem 2.3 gives

$$\begin{vmatrix} X \\ Y \end{vmatrix} = \begin{vmatrix} Y \\ X \end{vmatrix} \quad \text{and} \quad \begin{vmatrix} X_1, X_2 \\ Y_1, Y_2 \end{vmatrix} = \begin{vmatrix} Y_1 + Y_2, Y_1 \\ X_2, X_1 - X_2 \end{vmatrix}.$$

The statement follows by considering the coefficients of $X^{s-1}Y^r$ and $X_1^{s_1-1}X_2^{s_2-1}Y^{r_1}Y^{r_2}$ in these equations. \square

Example 2.6. i) Some examples for the length two case:

$$\begin{aligned} \begin{bmatrix} 1, 1 \\ 1, 1 \end{bmatrix} &= \begin{bmatrix} 2, 2 \\ 0, 0 \end{bmatrix} + 2 \begin{bmatrix} 3, 1 \\ 0, 0 \end{bmatrix}, & \begin{bmatrix} 3, 3 \\ 0, 0 \end{bmatrix} &= 6 \begin{bmatrix} 1, 1 \\ 0, 4 \end{bmatrix} - 3 \begin{bmatrix} 1, 1 \\ 1, 3 \end{bmatrix} + \begin{bmatrix} 1, 1 \\ 2, 2 \end{bmatrix}, \\ \begin{bmatrix} 2, 2 \\ 1, 1 \end{bmatrix} &= -2 \begin{bmatrix} 2, 2 \\ 0, 2 \end{bmatrix} + \begin{bmatrix} 2, 2 \\ 1, 1 \end{bmatrix} - 4 \begin{bmatrix} 3, 1 \\ 0, 2 \end{bmatrix} + 2 \begin{bmatrix} 3, 1 \\ 1, 1 \end{bmatrix}, \\ \begin{bmatrix} 1, 2 \\ 2, 3 \end{bmatrix} &= - \begin{bmatrix} 4, 3 \\ 0, 1 \end{bmatrix} + \begin{bmatrix} 4, 3 \\ 1, 0 \end{bmatrix} - 4 \begin{bmatrix} 5, 2 \\ 0, 1 \end{bmatrix} + 4 \begin{bmatrix} 5, 2 \\ 1, 0 \end{bmatrix} - 10 \begin{bmatrix} 6, 1 \\ 0, 1 \end{bmatrix} + 10 \begin{bmatrix} 6, 1 \\ 1, 0 \end{bmatrix}. \end{aligned}$$

ii) Another family of relations which can be obtained by the partition relation is

$$\begin{bmatrix} \{1\}^n \\ \{0\}^{j-1}, 1, \{0\}^{n-j} \end{bmatrix} = \sum_{k=1}^{n-j+1} [\{1\}^{k-1}, 2, \{1\}^{n-k}]$$

for $1 \leq j \leq n$. For example:

$$\begin{bmatrix} 1 \\ 1 \end{bmatrix} = [2], \quad \begin{bmatrix} 1, 1, 1 \\ 0, 1, 0 \end{bmatrix} = [1, 2, 1] + [2, 1, 1].$$

Remark 2.7. We end the discussion on bi-brackets and their generating series by interpreting the coefficients of the bi-brackets as weighted sums over partitions which gives an natural explanation for the partition relation (2.1). By a partition of a natural number n with l parts we denote a representation of n as a sum of l distinct natural numbers, i.e. $15 = 4 + 4 + 3 + 2 + 1 + 1$ is a partition of 15 with the 4 parts given by 4, 3, 2, 1. We identify such a partition with a tuple $(u, v) \in \mathbb{N}^l \times \mathbb{N}^l$ where the u_j 's are the l distinct numbers in the partition and the v_j 's count their appearance in the sum.

The above partition of 15 is therefore given by the tuple $(u, v) = ((4, 3, 2, 1), (2, 1, 1, 2))$. By $P_l(n)$ we denote all partitions of n with l parts and hence we set

$$P_l(n) := \left\{ (u, v) \in \mathbb{N}^l \times \mathbb{N}^l \mid n = u_1 v_1 + \cdots + u_l v_l \text{ and } u_1 > \cdots > u_l > 0 \right\}$$

On the set $P_l(n)$ one has an involution given by the conjugation ρ of partitions which can be obtained by reflecting the corresponding Young diagram across the main diagonal. On the set $P_l(n)$ the conjugation ρ is explicitly given by $\rho((u, v)) = (u', v')$ where

$$((4, 3, 2, 1), (2, 1, 1, 2)) = \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & & \\ \hline \square & & & \\ \hline \square & & & \\ \hline \end{array} \xrightarrow{\rho} \begin{array}{|c|c|c|c|c|} \hline \square & \square & \square & \square & \square \\ \hline \square & \square & & & \\ \hline \square & & & & \\ \hline \square & & & & \\ \hline \square & & & & \\ \hline \end{array} = ((6, 4, 3, 2), (1, 1, 1, 1))$$

Figure 1: The conjugation of the partition $15 = 4 + 4 + 3 + 2 + 1 + 1$ is given by $\rho(((4, 3, 2, 1), (2, 1, 1, 2))) = ((6, 4, 3, 2), (1, 1, 1, 1))$ which can be seen by reflection the corresponding Young diagram at the main diagonal.

$u'_j = v_1 + \cdots + v_{l-j+1}$ and $v'_j = u_{l-j+1} - u_{l-j+2}$ with $u_{l+1} := 0$, i.e.

$$\rho : \begin{pmatrix} u_1, \dots, u_l \\ v_1, \dots, v_l \end{pmatrix} \mapsto \begin{pmatrix} v_1 + \cdots + v_l, \dots, v_1 + v_2, v_1 \\ u_l, u_{l-1} - u_l, \dots, u_1 - u_2 \end{pmatrix}. \quad (2.2)$$

By the definition of the bi-brackets its clear that with the above notation they can be written as

$$\left[\begin{array}{c} s_1, \dots, s_l \\ r_1, \dots, r_l \end{array} \right] := \frac{1}{r_1!(s_1 - 1)! \cdots r_l!(s_l - 1)!} \sum_{n>0} \left(\sum_{(u,v) \in P_l(n)} u_1^{r_1} v_1^{s_1-1} \cdots u_l^{r_l} v_l^{s_l-1} \right) q^n.$$

The coefficients are given by a sum over all elements in $P_l(n)$ and therefore it is invariant under the action of ρ . As an example consider $[2, 2]$ and apply ρ to the sum then we obtain

$$\begin{aligned} [2, 2] &= \sum_{n>0} \left(\sum_{(u,v) \in P_2(n)} v_1 \cdot v_2 \right) q^n = \sum_{n>0} \left(\sum_{\rho((u,v)) = (u',v') \in P_2(n)} u'_2 \cdot (u'_1 - u'_2) \right) q^n \\ &= \sum_{n>0} \left(\sum_{(u',v') \in P_2(n)} u'_2 \cdot u'_1 \right) q^n - \sum_{n>0} \left(\sum_{(u',v') \in P_2(n)} u'^2_2 \right) q^n = \begin{bmatrix} 1, 1 \\ 1, 1 \end{bmatrix} - 2 \begin{bmatrix} 1, 1 \\ 0, 2 \end{bmatrix}. \end{aligned} \quad (2.3)$$

This is exactly the relation one obtains by using the partition relation. Another trivial connection to partitions is given by the following: The coefficients of the brackets of the form $[\{1\}^l]$ count the number of partitions of length l . Summing over all length one therefore obtains the generating functions of all partitions:

$$\sum_{l>0} [\{1\}^l] = \sum_{n>0} p(n) q^n = \prod_{k=1}^{\infty} \frac{1}{1 - q^k}.$$

3 The algebra of bi-brackets

The partition relations give relations in a fixed length. To obtain relations with mixed length we need to consider the algebra structure on the space \mathcal{BD} . For this we first consider the product of bi-brackets in length one and then use the algebraic setup of quasi-shuffle algebras for the arbitrary length case.

Lemma 3.1. Let B_k be the k -th Bernoulli number, then we get for all $n \in \mathbb{N}$

$$L_n(X) \cdot L_n(Y) = \sum_{k>0} \frac{B_k}{k!} (X - Y)^{k-1} L_n(X) + \sum_{k>0} \frac{B_k}{k!} (Y - X)^{k-1} L_n(Y) + \frac{L_n(X) - L_n(Y)}{X - Y}.$$

Proof. By direct computations one obtains

$$L(X) \cdot L(Y) = \frac{1}{e^{X-Y} - 1} L(X) + \frac{1}{e^{Y-X} - 1} L(Y).$$

The statement follows then by the definition of the Bernoulli numbers

$$\frac{X}{e^X - 1} = \sum_{n \geq 0} \frac{B_n}{n!} X^n.$$

□

Lemma 3.2. The product of two generating functions in length one can be written as

i) ("Stuffle product for bi-brackets")

$$\begin{aligned} \left| \begin{array}{c} X_1 \\ Y_1 \end{array} \right| \cdot \left| \begin{array}{c} X_2 \\ Y_2 \end{array} \right| &= \left| \begin{array}{c} X_1, X_2 \\ Y_1, Y_2 \end{array} \right| + \left| \begin{array}{c} X_2, X_1 \\ Y_2, Y_1 \end{array} \right| + \frac{1}{X_1 - X_2} \left(\left| \begin{array}{c} X_1 \\ Y_1 + Y_2 \end{array} \right| - \left| \begin{array}{c} X_2 \\ Y_1 + Y_2 \end{array} \right| \right) \\ &+ \sum_{k=1}^{\infty} \frac{B_k}{k!} (X_1 - X_2)^{k-1} \left(\left| \begin{array}{c} X_1 \\ Y_1 + Y_2 \end{array} \right| + (-1)^{k-1} \left| \begin{array}{c} X_2 \\ Y_1 + Y_2 \end{array} \right| \right). \end{aligned}$$

ii) ("Shuffle product for bi-brackets")

$$\begin{aligned} \left| \begin{array}{c} X_1 \\ Y_1 \end{array} \right| \cdot \left| \begin{array}{c} X_2 \\ Y_2 \end{array} \right| &= \left| \begin{array}{c} X_1 + X_2, X_1 \\ Y_2, Y_1 - Y_2 \end{array} \right| + \left| \begin{array}{c} X_1 + X_2, X_2 \\ Y_1, Y_2 - Y_1 \end{array} \right| + \frac{1}{Y_1 - Y_2} \left(\left| \begin{array}{c} X_1 + X_2 \\ Y_1 \end{array} \right| - \left| \begin{array}{c} X_1 + X_2 \\ Y_2 \end{array} \right| \right) \\ &+ \sum_{k=1}^{\infty} \frac{B_k}{k!} (Y_1 - Y_2)^{k-1} \left(\left| \begin{array}{c} X_1 + X_2 \\ Y_1 \end{array} \right| + (-1)^{k-1} \left| \begin{array}{c} X_1 + X_2 \\ Y_2 \end{array} \right| \right) \end{aligned}$$

Proof. We prove *i)* and *ii)* by using the two different ways of writing the generating functions given by Theorem 2.3.

i) By direct calculation it is

$$\left| \begin{array}{c} X_1 \\ Y_1 \end{array} \right| \cdot \left| \begin{array}{c} X_2 \\ Y_2 \end{array} \right| = \left| \begin{array}{c} X_1, X_2 \\ Y_1, Y_2 \end{array} \right| + \left| \begin{array}{c} X_2, X_1 \\ Y_2, Y_1 \end{array} \right| + \sum_{n>0} E_n(Y_1 + Y_2) L_n(X_1) L_n(X_2).$$

Applying the Lemma 3.1 to the last term yields the statement.

ii) The partition relation in length one and two (P) in (2.1) states

$$\left| \begin{array}{c} X_1 \\ Y_1 \end{array} \right| \stackrel{P}{=} \left| \begin{array}{c} Y_1 \\ X_1 \end{array} \right|, \quad \left| \begin{array}{c} X_1, X_2 \\ Y_1, Y_2 \end{array} \right| \stackrel{P}{=} \left| \begin{array}{c} Y_1 + Y_2, Y_1 \\ X_2, X_1 - X_2 \end{array} \right|,$$

and together with i) we obtain

$$\begin{aligned} \left| \begin{array}{c} X_1 \\ Y_1 \end{array} \right| \cdot \left| \begin{array}{c} X_2 \\ Y_2 \end{array} \right| &\stackrel{P}{=} \left| \begin{array}{c} Y_1 \\ X_1 \end{array} \right| \cdot \left| \begin{array}{c} Y_2 \\ X_2 \end{array} \right| \stackrel{i)}{=} \left| \begin{array}{c} Y_1, Y_2 \\ X_1, X_2 \end{array} \right| + \left| \begin{array}{c} Y_2, Y_1 \\ X_2, X_1 \end{array} \right| + \frac{1}{Y_1 - Y_2} \left(\left| \begin{array}{c} Y_1 \\ X_1 + X_2 \end{array} \right| - \left| \begin{array}{c} Y_2 \\ X_1 + X_2 \end{array} \right| \right) \\ &+ \sum_{k=1}^{\infty} \frac{B_k}{k!} (Y_1 - Y_2)^{k-1} \left(\left| \begin{array}{c} Y_1 \\ X_1 + X_2 \end{array} \right| + (-1)^{k-1} \left| \begin{array}{c} Y_2 \\ X_1 + X_2 \end{array} \right| \right) \\ &\stackrel{P}{=} \left| \begin{array}{c} X_1 + X_2, X_1 \\ Y_2, Y_1 - Y_2 \end{array} \right| + \left| \begin{array}{c} X_1 + X_2, X_2 \\ Y_1, Y_2 - Y_1 \end{array} \right| + \frac{1}{Y_1 - Y_2} \left(\left| \begin{array}{c} X_1 + X_2 \\ Y_1 \end{array} \right| - \left| \begin{array}{c} X_1 + X_2 \\ Y_2 \end{array} \right| \right) \\ &+ \sum_{k=1}^{\infty} \frac{B_k}{k!} (Y_1 - Y_2)^{k-1} \left(\left| \begin{array}{c} X_1 + X_2 \\ Y_1 \end{array} \right| + (-1)^{k-1} \left| \begin{array}{c} X_1 + X_2 \\ Y_2 \end{array} \right| \right). \end{aligned}$$

□

Proposition 3.3. For $s_1, s_2 > 0$ and $r_1, r_2 \geq 0$ we have the following two expressions for the product of two bi-brackets of length one:

i) ("Stuffle product for bi-brackets")

$$\begin{aligned} \begin{bmatrix} s_1 \\ r_1 \end{bmatrix} \cdot \begin{bmatrix} s_2 \\ r_2 \end{bmatrix} &= \begin{bmatrix} s_1, s_2 \\ r_1, r_2 \end{bmatrix} + \begin{bmatrix} s_2, s_1 \\ r_2, r_1 \end{bmatrix} + \binom{r_1 + r_2}{r_1} \begin{bmatrix} s_1 + s_2 \\ r_1 + r_2 \end{bmatrix} \\ &+ \binom{r_1 + r_2}{r_1} \sum_{j=1}^{s_1} \frac{(-1)^{s_2-1} B_{s_1+s_2-j}}{(s_1 + s_2 - j)!} \binom{s_1 + s_2 - j - 1}{s_1 - j} \begin{bmatrix} j \\ r_1 + r_2 \end{bmatrix} \\ &+ \binom{r_1 + r_2}{r_1} \sum_{j=1}^{s_2} \frac{(-1)^{s_1-1} B_{s_1+s_2-j}}{(s_1 + s_2 - j)!} \binom{s_1 + s_2 - j - 1}{s_2 - j} \begin{bmatrix} j \\ r_1 + r_2 \end{bmatrix} \end{aligned}$$

ii) ("Shuffle product for bi-brackets")

$$\begin{aligned}
\begin{bmatrix} s_1 \\ r_1 \end{bmatrix} \cdot \begin{bmatrix} s_2 \\ r_2 \end{bmatrix} &= \sum_{\substack{1 \leq j \leq s_1 \\ 0 \leq k \leq r_2}} \binom{s_1 + s_2 - j - 1}{s_1 - j} \binom{r_1 + r_2 - k}{r_1} (-1)^{r_2 - k} \begin{bmatrix} s_1 + s_2 - j, j \\ k, r_1 + r_2 - k \end{bmatrix} \\
&+ \sum_{\substack{1 \leq j \leq s_2 \\ 0 \leq k \leq r_1}} \binom{s_1 + s_2 - j - 1}{s_1 - 1} \binom{r_1 + r_2 - k}{r_1 - k} (-1)^{r_1 - k} \begin{bmatrix} s_1 + s_2 - j, j \\ k, r_1 + r_2 - k \end{bmatrix} \\
&+ \binom{s_1 + s_2 - 2}{s_1 - 1} \begin{bmatrix} s_1 + s_2 - 1 \\ r_1 + r_2 + 1 \end{bmatrix} \\
&+ \binom{s_1 + s_2 - 2}{s_1 - 1} \sum_{j=0}^{r_1} \frac{(-1)^{r_2} B_{r_1 + r_2 - j + 1}}{(r_1 + r_2 - j + 1)!} \binom{r_1 + r_2 - j}{r_1 - j} \begin{bmatrix} s_1 + s_2 - 1 \\ j \end{bmatrix} \\
&+ \binom{s_1 + s_2 - 2}{s_1 - 1} \sum_{j=0}^{r_2} \frac{(-1)^{r_1} B_{r_1 + r_2 - j + 1}}{(r_1 + r_2 - j + 1)!} \binom{r_1 + r_2 - j}{r_2 - j} \begin{bmatrix} s_1 + s_2 - 1 \\ j \end{bmatrix}
\end{aligned}$$

Proof. i) By Lemma 3.2 it is

$$\begin{aligned}
\begin{vmatrix} X_1 \\ Y_1 \end{vmatrix} \cdot \begin{vmatrix} X_2 \\ Y_2 \end{vmatrix} &= \underbrace{\begin{vmatrix} X_1, X_2 \\ Y_1, Y_2 \end{vmatrix} + \begin{vmatrix} X_2, X_1 \\ Y_2, Y_1 \end{vmatrix}}_{=:T_1} + \underbrace{\frac{1}{X_1 - X_2} \left(\begin{vmatrix} X_1 \\ Y_1 + Y_2 \end{vmatrix} - \begin{vmatrix} X_2 \\ Y_1 + Y_2 \end{vmatrix} \right)}_{=:T_2} \\
&+ \underbrace{\sum_{k=1}^{\infty} \frac{B_k}{k!} (X_1 - X_2)^{k-1} \left(\begin{vmatrix} X_1 \\ Y_1 + Y_2 \end{vmatrix} + (-1)^{k-1} \begin{vmatrix} X_2 \\ Y_1 + Y_2 \end{vmatrix} \right)}_{=:T_3}.
\end{aligned}$$

We are going to calculate the coefficient of $X^{s_1 - 1} X_2^{s_2 - 1} Y_1^{r_1} Y_2^{r_2}$ in this equation. Clearly $\begin{bmatrix} s_1, s_2 \\ r_1, r_2 \end{bmatrix} + \begin{bmatrix} s_2, s_1 \\ r_2, r_1 \end{bmatrix}$ is the coefficient of T_1 and by the use of

$$\sum_{s>0} c_s \frac{X_1^{s-1} - X_2^{s-1}}{X_1 - X_2} = \sum_{s>0} c_s \sum_{j=0}^{s-2} X_1^{s-2-j} X_2^j = \sum_{a,b>0} c_{a+b} X_1^{a-1} X_2^{b-1}$$

one obtains

$$\begin{aligned}
T_2 &= \frac{1}{X_1 - X_2} \left(\begin{vmatrix} X_1 \\ Y_1 + Y_2 \end{vmatrix} - \begin{vmatrix} X_2 \\ Y_1 + Y_2 \end{vmatrix} \right) = \sum_{s_1, s_2, r > 0} \begin{bmatrix} s_1 + s_2 \\ r - 1 \end{bmatrix} X_1^{s_1 - 1} X_2^{s_2 - 1} (Y_1 + Y_2)^{r-1} \\
&= \sum_{\substack{s_1, s_2 > 0 \\ r_1, r_2 > 0}} \binom{r_1 + r_2 - 2}{r_1 - 1} \begin{bmatrix} s_1 + s_2 \\ r_1 + r_2 - 2 \end{bmatrix} X_1^{s_1 - 1} X_2^{s_2 - 1} Y_1^{r_1 - 1} Y_2^{r_2 - 1}.
\end{aligned}$$

With a bit more tedious but similar calculation one shows that the remaining terms are the coefficients of T_3 .

ii) This statement follows by a similar calculation as in i). □

We now want to recall the algebraic setting of Hoffman for quasi-shuffle products and give the necessary notations for the rest of the paper.

Definition 3.4. Let A (the alphabet) be a countable set of letters, $\mathbb{Q}A$ the \mathbb{Q} -vector space generated by these letters and $\mathbb{Q}\langle A \rangle$ the noncommutative polynomial algebra over \mathbb{Q} generated by words with letters in A . For a commutative and associative product \diamond on $\mathbb{Q}A$, $a, b \in A$ and $w, v \in \mathbb{Q}\langle A \rangle$ we define on $\mathbb{Q}\langle A \rangle$ recursively a product by $1 \odot w = w \odot 1 = w$ and

$$aw \odot bv := a(w \odot bv) + b(aw \odot v) + (a \diamond b)(w \odot v). \quad (3.1)$$

By a result of Hoffman ([H]) $(\mathbb{Q}\langle A \rangle, \odot)$ is a commutative \mathbb{Q} -algebra which is called a *quasi-shuffle algebra*.

Notation 3.5. Let us now recall some basic notations for the shuffle and the stuffle product which are the easiest examples of quasi-shuffle products. Since we will deal with the shuffle product for different alphabets simultaneously we will use some additional notations for this. For the alphabet $A_{xy} := \{x, y\}$ set $\mathfrak{H} = \mathbb{Q}\langle A_{xy} \rangle$ and $\mathfrak{H}^1 = 1 \cdot \mathbb{Q} + \mathfrak{H}y$, with 1 being the empty word. It is easy to see that \mathfrak{H}^1 is generated by the elements $z_j = x^{j-1}y$ with $j \in \mathbb{N}$, i.e. $\mathfrak{H}^1 = \mathbb{Q}\langle A_z \rangle$ with $A_z := \{z_1, z_2, \dots\}$. By $|w|$ we denote the weight of a word $w \in \mathfrak{H}$ which is given by the number of letters (in the alphabet A_{xy}) of w . On \mathfrak{H}^1 we have the following two products with respect to the alphabet A_z which we call the *index-shuffle*, denoted by \sqcup with $\diamond \equiv 0$, and the *stuffle product*, denoted by $*$ with $z_j \diamond z_i = z_{j+i}$, i.e. we have for $a, b \in \mathbb{N}$ and $w, v \in \mathfrak{H}^1$:

$$\begin{aligned} z_a w \sqcup z_b v &= z_a(w \sqcup z_b v) + z_b(z_a w \sqcup v), \\ z_a w * z_b v &= z_a(w * z_b v) + z_b(z_a w * v) + z_{a+b}(w * v). \end{aligned} \quad (3.2)$$

By $(\mathfrak{H}_z^1, \sqcup)$ and $(\mathfrak{H}_z^1, *)$ we denote the corresponding \mathbb{Q} -algebras, where the subscript z indicates that we consider the quasi-shuffle with respect to the alphabet A_z . We can also define the shuffle product on \mathfrak{H}^1 with respect to the alphabet A_{xy} , which we call the *shuffle product*, and by $(\mathfrak{H}_{xy}^1, \sqcup)$ we denote the corresponding \mathbb{Q} -algebra.

We now want to find a \diamond and a suitable alphabet such that we can view the algebra of bi-brackets as a quasi-shuffle algebra. For $a, b \in \mathbb{N}$ define the numbers $\lambda_{a,b}^j \in \mathbb{Q}$ for $1 \leq j \leq a$ as

$$\lambda_{a,b}^j = (-1)^{b-1} \binom{a+b-j-1}{a-j} \frac{B_{a+b-j}}{(a+b-j)!}.$$

For the alphabet $A_z^{\text{bi}} := \{z_{s,r} \mid s, r \in \mathbb{Z}, s \geq 1, r \geq 0\}$ we define on $\mathbb{Q}A_z^{\text{bi}}$ the product

$$\begin{aligned} z_{s_1, r_1} \boxtimes z_{s_2, r_2} &= \binom{r_1 + r_2}{r_1} \sum_{j=1}^{s_1} \lambda_{s_1, s_2}^j z_{j, r_1 + r_2} + \binom{r_1 + r_2}{r_1} \sum_{j=1}^{s_2} \lambda_{s_2, s_1}^j z_{j, r_1 + r_2} \\ &\quad + \binom{r_1 + r_2}{r_1} z_{s_1 + s_2, r_1 + r_2} \end{aligned}$$

and on $\mathbb{Q}\langle A_z^{\text{bi}} \rangle$ the quasi-shuffle product

$$z_{s_1, r_1} w \boxtimes z_{s_2, r_2} v = z_{s_1, r_1} (w \boxtimes z_{s_2, r_2} v) + z_{s_2, r_2} (z_{s_1, r_1} w \boxtimes v) + (z_{s_1, r_1} \boxtimes z_{s_2, r_2})(w \boxtimes v).$$

Theorem 3.6. i) The product \boxtimes on $\mathbb{Q}A_z^{\text{bi}}$ is associative and therefore $(\mathbb{Q}\langle A_z^{\text{bi}} \rangle, \boxtimes)$ is a quasi-shuffle Algebra.

ii) The map $[\cdot] : (\mathbb{Q}\langle A_z^{\text{bi}} \rangle, \boxtimes) \rightarrow (\mathcal{BD}, \cdot)$ given by

$$w = z_{s_1, r_1} \dots z_{s_l, r_l} \mapsto [w] = \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix}$$

fulfills $[w \boxtimes v] = [w] \cdot [v]$ and therefore \mathcal{BD} is a \mathbb{Q} -algebra.

Proof. Using Proposition 2.3 in [BK] it is easy to see that

$$\begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} = \sum_{u_1 > \dots > u_l > 0} \frac{u_1^{r_1}}{r_1!} \tilde{\text{Li}}_{s_1}(q^{u_1}) \dots \frac{u_l^{r_l}}{r_l!} \tilde{\text{Li}}_{s_l}(q^{u_l}), \quad (3.3)$$

where $\tilde{\text{Li}}_s(x) = \frac{\text{Li}_{1-s}(x)}{(s-1)!}$. Due to Lemma 3.1 (see also Lemma 2.5 in [BK]) we have

$$\tilde{\text{Li}}_a(z) \cdot \tilde{\text{Li}}_b(z) = \sum_{j=1}^a \lambda_{a,b}^j \tilde{\text{Li}}_j(z) + \sum_{j=1}^b \lambda_{b,a}^j \tilde{\text{Li}}_j(z) + \tilde{\text{Li}}_{a+b}(z),$$

This proves the first statement and the second statement follows directly by the definition of \boxtimes . \square

Remark 3.7. As we saw in the proof of Proposition 3.2 for the product of two length one bi-brackets, the shuffle product of bi-brackets is obtained by applying the partition relation, the stuffle product and again the partition relation. This of course works for arbitrary lengths and yields a natural way to obtain the shuffle product for bi-brackets. To make this precise denote by $P : \mathbb{Q}\langle A_z^{\text{bi}} \rangle \rightarrow \mathbb{Q}\langle A_z^{\text{bi}} \rangle$ the linearly extended map which sends a word $w = z_{s_1, r_1} \dots z_{s_l, r_l}$ to the linear combination of words corresponding to the partition relation. Using this convention the shuffle product for brackets can be written in $\mathbb{Q}\langle A_z^{\text{bi}} \rangle$ for two words $u, v \in \mathbb{Q}\langle A_z^{\text{bi}} \rangle$ as $P(P(u) \boxtimes P(v))$, i.e. the stuffle and shuffle product for bi-brackets can be written as

$$[u] \cdot [v] \stackrel{st}{=} [u \boxtimes v], \quad [u] \cdot [v] \stackrel{sh}{=} [P(P(u) \boxtimes P(v))]. \quad (3.4)$$

Remark 3.8. As mentioned in the introduction the bi-brackets can be seen as a q -analogue of MZV: Define for $k \in \mathbb{N}$ the map $\mathbb{Q}[[q]] \rightarrow \mathbb{R} \cup \{\infty\}$ by $Z_k(f) = \lim_{q \rightarrow 1} (1 - q)^k f(q)$, which was introduced and discussed in [BK] for the subspace $\mathcal{MD} \subset \mathbb{Q}[[q]]$. On the bi-brackets this map is given by the following: Assume that $s_1 > r_1 + 1$ and

$s_j \geq r_j + 1$ for $j = 2, \dots, l$, then, using the description (3.3) (see eg. Proposition 1 in [Zu]), we obtain

$$Z_{s_1+\dots+s_l} \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} = \frac{1}{r_1! \dots r_l!} \zeta(s_1 - r_1, \dots, s_l - r_l).$$

Even though we don't want to discuss this issue in this note it is worth mentioning that an other motivation for considering the bi-brackets was to describe the kernel of the map Z_k on the space $\text{gr}_k^{\text{W}} \mathcal{MD}$. This connection will be subject of upcoming works. Applying the map Z_k to the equation (3.4) one obtains the stuffle and shuffle product formula for MZV (See [Zu]). Finally we want mention that there are several other different types of q -analogues which also have a stuffle and shuffle like structure (See for example [MMEF] and [Zh] for a nice overview).

4 Derivatives and modular forms

In this section we want to discuss derivatives of bi-brackets with respect to the differential operator $q \frac{d}{dq}$ and their connections to modular forms. For this we first introduce the following notations:

Definition 4.1. On \mathcal{BD} we have the increasing filtrations $\text{Fil}_\bullet^{\text{W}}$ given by the upper weight, $\text{Fil}_\bullet^{\text{D}}$ give by the lower weight and $\text{Fil}_\bullet^{\text{L}}$ given by the length, i.e., we have for $A \subseteq \mathcal{BD}$

$$\begin{aligned} \text{Fil}_k^{\text{W}}(A) &:= \left\langle \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \in A \mid 0 \leq l \leq k, s_1 + \dots + s_l \leq k \right\rangle_{\mathbb{Q}} \\ \text{Fil}_k^{\text{D}}(A) &:= \left\langle \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} \in A \mid 0 \leq l \leq k, r_1 + \dots + r_l \leq k \right\rangle_{\mathbb{Q}} \\ \text{Fil}_l^{\text{L}}(A) &:= \left\langle \begin{bmatrix} s_1, \dots, s_t \\ r_1, \dots, r_t \end{bmatrix} \in A \mid t \leq l \right\rangle_{\mathbb{Q}}. \end{aligned}$$

If we consider the length and weight filtration at the same time we use the short notation $\text{Fil}_{k,l}^{\text{W,L}} := \text{Fil}_k^{\text{W}} \text{Fil}_l^{\text{L}}$ and similar for the other filtrations.

Proposition 4.2. Let $d_q := q \frac{d}{dq}$ then we have

$$d_q \begin{bmatrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{bmatrix} = \sum_{j=1}^l \left(s_j(r_j + 1) \begin{bmatrix} s_1, \dots, s_{j-1}, s_j + 1, s_{j+1}, \dots, s_l \\ r_1, \dots, r_{j-1}, r_j + 1, r_{j+1}, \dots, r_l \end{bmatrix} \right)$$

and therefore $d_q \left(\text{Fil}_{k,d,l}^{\text{W,D,L}}(\mathcal{BD}) \right) \subset \text{Fil}_{k+1,d+1,l}^{\text{W,D,L}}(\mathcal{BD})$.

Proof. This is an easy consequence of the definition of bi-brackets and the fact that $d_q \sum_{n>0} a_n q^n = \sum_{n>0} n a_n q^n$. Another way to see this is by the fact that the operator d_q on the generating series of bi-brackets can be written as

$$d_q \left| \begin{array}{c} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{array} \right| = \sum_{j=1}^l \frac{\partial}{\partial X_j} \frac{\partial}{\partial Y_j} \left| \begin{array}{c} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{array} \right|,$$

which follows from

$$d_q E_n(Y) L_n(X) = d_q \frac{e^{nY} e^X q^n}{(1 - e^X q^n)} = \frac{n e^{nY} e^X q^n}{(1 - e^X q^n)^2} = \frac{\partial}{\partial X} \frac{\partial}{\partial Y} E_n(Y) L_n(X).$$

□

Proposition 4.2 suggests that the bi-brackets can be somehow viewed as partial derivatives of the brackets with total differential d_q . In this part we want to give some explicit results on the following conjecture which was inspired by numerical experiments and which, with the above interpretation, states that the space \mathcal{MD} is closed under partial derivatives.

Conjecture 4.3. The algebra \mathcal{BD} of bi-brackets is a subalgebra of \mathcal{MD} and in particular we have

$$\text{Fil}_{k,d,l}^{\text{W,D,L}}(\mathcal{BD}) \subset \text{Fil}_{k+d,l+d}^{\text{W,L}}(\mathcal{MD}).$$

Proposition 4.4. For $l = 1$ the conjecture 4.3 is true.

Proof. In [BK] the authors proved that $d_q \mathcal{MD} \subset \mathcal{MD}$. Due to Proposition 4.2 we therefore have $\left[\begin{smallmatrix} s \\ r \end{smallmatrix} \right] \in \mathcal{MD}$, i.e. the Conjecture is true for the length one case. □

Remark 4.5. In [BK2] it will be shown that up to weight $k \leq 7$ every bi-bracket can be written in terms of brackets, by giving upper bounds for the number of algebra generators of bi-brackets.

For lower weight $d = 1$ Proposition 4.4 is given explicitly by the following reformulation of Proposition 3.3 in [BK].

Proposition 4.6. For all $k \geq 1$ it is

$$\begin{aligned} \left[\begin{array}{c} k \\ 1 \end{array} \right] &= [k] \cdot [1] - \sum_{a+b=k+1} [a, b] - [k, 1] + [k] \\ &= [k+1] + \frac{1}{2}[k] - \sum_{\substack{a+b=k+1 \\ a>1}} [a, b] + \sum_{j=2}^{k-1} \frac{B_{k-j+1}}{(k-j+1)!} [j] - \frac{1}{2} \delta_{k,1} [1] \in \text{Fil}_{k+1,2}^{\text{W,L}}(\mathcal{MD}) \end{aligned}$$

Proof. The functions $L_n(X)$ in the generating function fulfil the following differential equation.

$$\frac{\partial}{\partial X} L_n(X) = L_n(X)^2 + L_n(X).$$

Therefore we get

$$\frac{\partial}{\partial Y} \left| \begin{array}{c} X \\ Y \end{array} \right| = \sum_{n>0} e^{nX} L_n(Y)^2 + \sum_{n>0} e^{nX} L_n(Y) = \sum_{n>0} e^{nX} L_n(Y)^2 + \left| \begin{array}{c} X \\ Y \end{array} \right|.$$

The first term also appears in the product of two generating functions:

$$\begin{aligned} \left| \begin{array}{c} X \\ Y \end{array} \right| \cdot \left| \begin{array}{c} 0 \\ Y \end{array} \right| &= \sum_{n_1>n_2>0} e^{n_1X} L_{n_1}(Y) L_{n_2}(Y) + \sum_{n_2>n_1>0} e^{n_1X} L_{n_1}(Y) L_{n_2}(Y) + \sum_{n>0} e^{nX} L_n(Y)^2 \\ &= \left| \begin{array}{c} Y, Y \\ X, 0 \end{array} \right| + \left| \begin{array}{c} Y, Y \\ 0, X \end{array} \right| + \sum_{n>0} e^{nX} L_n(Y)^2 = \left| \begin{array}{c} X, X \\ Y, 0 \end{array} \right| + \left| \begin{array}{c} X, 0 \\ Y, 0 \end{array} \right| + \sum_{n>0} e^{nX} L_n(Y)^2. \end{aligned}$$

And therefore we obtain

$$\frac{\partial}{\partial Y} \left| \begin{array}{c} X \\ Y \end{array} \right| = \left| \begin{array}{c} X \\ Y \end{array} \right| \cdot \left| \begin{array}{c} 0 \\ Y \end{array} \right| - \left| \begin{array}{c} X, X \\ Y, 0 \end{array} \right| - \left| \begin{array}{c} X, 0 \\ Y, 0 \end{array} \right| + \left| \begin{array}{c} X \\ Y \end{array} \right|, \quad (4.1)$$

which gives the first expression by considering the coefficient of X^{k-1} in this equation. The second statement follows from the explicit stuffle product for bi-brackets in Proposition 3.3:

$$[k] \cdot [1] = [k, 1] + [1, k] + [k + 1] + \sum_{j=2}^k \frac{B_{k-j+1}}{(k-j+1)!} [j] - \delta_{k,1}[1].$$

□

There it not much known so far for the length two and arbitrary weight case of the Conjecture 4.3. Using the shuffle brackets we will prove (see Proposition 5.9) that for all $s_1, s_2 \geq 1$ it is

$$\left[\begin{array}{c} s_1, s_2 \\ 1, 0 \end{array} \right], \left[\begin{array}{c} s_1, s_2 \\ 0, 1 \end{array} \right] \in \text{Fil}_{s_1+s_2+1,3}^{\text{W,L}}(\mathcal{MD})$$

It would be interesting to know whether the approach in the proof of proposition 5.9 also works for higher lengths, or higher lower weight.

One motivation of considering (bi-)brackets is to build a connection between multiple zeta values and modular forms. In the following we will show how to use the double shuffle structure on the space of bi-brackets described above to prove relations between modular forms. On the other hand we use results of modular forms to prove relations between bi-brackets. For $k \in \mathbb{N}$ denote by

$$\tilde{G}_k = \frac{\zeta(k)}{(-2\pi i)^k} + \frac{1}{(k-1)!} \sum_{n>0} \sigma_{k-1}(n) q^n = \frac{\zeta(k)}{(-2\pi i)^k} + [k].$$

the Eisenstein series of weight k . For even $k = 2n$ due to Euler we have $\zeta(2n) = \frac{(-1)^{n-1} B_{2n} (2\pi)^{2n}}{2(2n)!}$ and therefore $\tilde{G}_{2n} = -\frac{1}{2} \frac{B_{2n}}{(2n)!} + [2n] =: \beta_{2n} + [2n] \in \text{Fil}_{2n}^{\text{W}}(\mathcal{MD})$, for example

$$\tilde{G}_2 = -\frac{1}{24} + [2], \quad \tilde{G}_4 = \frac{1}{1440} + [4], \quad \tilde{G}_6 = -\frac{1}{60480} + [6].$$

Proposition 4.7. i) The ring of modular forms $M(\Gamma_1)$ for $\Gamma_1 = SL_2(\mathbb{Z})$ and the ring of quasi-modular forms $\tilde{M}(\Gamma_1)$ are graded subalgebras of \mathcal{MD} .

ii) The \mathbb{Q} -algebra of quasi-modular forms $\tilde{M}_k(\Gamma_1)$ is closed under the derivation d_q and therefore it is a subalgebra of the graded differential algebra (\mathcal{MD}, d_q) .

iii) We have the following inclusions of \mathbb{Q} -algebras

$$M_k(\Gamma_1) \subset \tilde{M}(\Gamma_1) \subset {}_q\mathcal{MZ} \subset \mathcal{MD} \subset \mathcal{BD}.$$

Proof. Let $M_k(\Gamma_1)$ (resp. $\tilde{M}_k(\Gamma_1)$) be the space of (quasi-)modular forms of weight k for Γ_1 . Then the first claim follows directly from the well-known facts $M(\Gamma_1) = \bigoplus_{k>1} M(\Gamma_1)_k = \mathbb{Q}[\tilde{G}_4, \tilde{G}_6]$ and $\tilde{M}(\Gamma_1) = \bigoplus_{k>1} \tilde{M}(\Gamma_1)_k = \mathbb{Q}[\tilde{G}_2, \tilde{G}_4, \tilde{G}_6]$. The second claim is a well known fact in the theory of quasi-modular forms and a proof can be found in [Za] p. 49. It suffices to show that the derivatives of the generators are given by

$$\begin{aligned} d_q \tilde{G}_2 &= d_q [2] = 5\tilde{G}_4 - 2\tilde{G}_2^2, & d_q \tilde{G}_4 &= 15\tilde{G}_6 - 8\tilde{G}_2\tilde{G}_4, \\ d_q \tilde{G}_6 &= 20\tilde{G}_8 - 12\tilde{G}_2\tilde{G}_6 = \frac{120}{7}\tilde{G}_4^2 - 12\tilde{G}_2\tilde{G}_6, \end{aligned}$$

which can be easily shown by the double shuffle relations of bi-brackets. \square

It is a well-known fact from the theory of modular forms that $\tilde{G}_4^2 = \frac{7}{6}\tilde{G}_8$ because the space of weight 8 modular forms for $SL_2(\mathbb{Z})$ is one dimensional. We therefore have

$$\frac{1}{720}[4] + [4] \cdot [4] = \frac{7}{6}[8].$$

Using the explicit stuffle product we get

$$[4] \cdot [4] = 2[4, 4] + [8] + \frac{1}{360}[4] - \frac{1}{1512}[2],$$

which then gives the following relation in $\text{Fil}_8^{\text{W}}(\mathcal{MD})$:

$$[8] = \frac{1}{40}[4] - \frac{1}{252}[2] + 12[4, 4]. \quad (4.2)$$

The identity (4.2) can also be proven by using the double shuffle relations, i.e. $\tilde{G}_4^2 = \frac{7}{6}G_8$ can be proven since it is equivalent to it. One can check that

$$\frac{1}{40}[4] - \frac{1}{252}[2] + 12[4, 4] - [8] = -4([3] \overset{st}{\cdot} [5] - [3] \overset{sh}{\cdot} [5]) + 3([4] \overset{st}{\cdot} [4] - [4] \overset{sh}{\cdot} [4]),$$

where the right hand side is clearly zero. This purely combinatorial approach to prove this kind of relation is similar to the one in [S].

Let us now use the theory of modular forms to obtain relations between bi-brackets. It is a well-known fact (see [Za] 5.2) that for two modular forms f and g of weight k and l the n th-Rankin-Cohen Bracket, where $n \geq 0$, given by

$$(f, g)_n = \sum_{\substack{a, b \geq 0 \\ a+b=n}} (-1)^a \binom{k+n-1}{b} \binom{l+n-1}{a} d_q^a f d_q^b g$$

is a modular form of weight $k+l+2n$. In the the case $n > 0$ this is a cusp form. For $f = \tilde{G}_k = \beta_k + [k]$ and $g = \tilde{G}_l = \beta_l + [l]$ we obtain by using $d_q^a \begin{bmatrix} k \\ 0 \end{bmatrix} = \frac{(k+a-1)! a!}{(k-1)!} \begin{bmatrix} k+a \\ a \end{bmatrix}$, that

$$(\tilde{G}_k, \tilde{G}_l)_n = \delta_{n,0} \beta_k \beta_l + \gamma_{k,l}^n \cdot C_{k,l}^{2n},$$

with $\gamma_{k,l}^n = \frac{(k-1+n)!}{(k-1)!} \cdot \frac{(l-1+n)!}{(l-1)!}$ and

$$C_{k,l}^{2n} = \beta_k \begin{bmatrix} l+n \\ n \end{bmatrix} + (-1)^n \beta_l \begin{bmatrix} k+n \\ n \end{bmatrix} + \sum_{\substack{a, b \geq 0 \\ a+b=n}} (-1)^a \begin{bmatrix} k+a \\ a \end{bmatrix} \begin{bmatrix} l+b \\ b \end{bmatrix}.$$

For all $n \geq 1$ and all even $k, l \geq 4$ the function $C_{k,l}^{2n} \in S_k$ is therefore a cusp form of weight $k+l+2n$. This yields a source for relations between bi-brackets since the dimension of S_k is smaller than the possible different $C_{k,l}^{2n}$. For example in weight 12 we have $\dim S_{12} = 1$ and we have the two expressions $\Delta = 12 \cdot 5!^2 \cdot C_{4,4}^4 = 5! \cdot 7! \cdot C_{4,6}^2$, with $\Delta = q \prod_{n \geq 0} (1 - q^n)^{24}$ being the unique normalized cusp form in this weight. This yields the following relations between bi-brackets

$$7 \begin{bmatrix} 5 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 6 \\ 0 \end{bmatrix} - 7 \begin{bmatrix} 4 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 7 \\ 1 \end{bmatrix} + 4 \begin{bmatrix} 4 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 6 \\ 2 \end{bmatrix} - 2 \begin{bmatrix} 5 \\ 1 \end{bmatrix} \cdot \begin{bmatrix} 5 \\ 1 \end{bmatrix} = \frac{7}{1440} \begin{bmatrix} 7 \\ 1 \end{bmatrix} - \frac{1}{360} \begin{bmatrix} 6 \\ 2 \end{bmatrix} + \frac{1}{8640} \begin{bmatrix} 5 \\ 1 \end{bmatrix}.$$

5 The spaces \mathcal{MD}^* and \mathcal{MD}^{\sqcup}

In [H] it is shown, that every quasi-shuffle Algebra $(\mathbb{Q}\langle A \rangle, \diamond)$ is isomorphic to the shuffle Algebra $(\mathbb{Q}\langle A \rangle, \sqcup)$. To make this precise define for a composition $i_1 + \dots + i_m = n$, where $i_1, \dots, i_m > 0$, of a natural number n and a word $w = a_1 a_2 \dots a_n$ the following element in $\mathbb{Q}\langle A \rangle$:

$$(i_1, \dots, i_m)\{w\} := (a_1 \diamond \dots \diamond a_{i_1})(a_{i_1+1} \diamond \dots \diamond a_{i_1+i_2}) \dots (a_{i_1+\dots+i_{m-1}+1} \diamond \dots \diamond a_n),$$

where the product is given by the composition of words and \diamond is the product on $\mathbb{Q}A$ belonging to \odot . With this define the following two maps

$$\begin{aligned}\exp_{\odot}(w) &= \sum_{\substack{1 \leq m \leq n \\ i_1 + \dots + i_m = n}} \frac{1}{i_1! \dots i_m!} (i_1, \dots, i_m) \{w\}, \\ \log_{\odot}(w) &= \sum_{\substack{1 \leq m \leq n \\ i_1 + \dots + i_m = n}} \frac{(-1)^{n-m}}{i_1 \dots i_m} (i_1, \dots, i_m) \{w\}.\end{aligned}$$

Proposition 5.1. ([H], Thm. 2.5) The map \exp_{\odot} is an algebra isomorphism from $(\mathbb{Q}\langle A \rangle, \sqcup)$ to $(\mathbb{Q}\langle A \rangle, \odot)$ with the inverse given by \log_{\odot} .

In other words this enables one to give an isomorphism between two arbitrary quasi-shuffle algebras on the same alphabets. We will use this now to define a stuffle version for the brackets and later on the generating series of bi-brackets to define the shuffle brackets.

Notice that for the brackets, i.e. bi-brackets with $r_1 = \dots = r_l = 0$, we also obtain an homomorphism $[\cdot] : (\mathfrak{H}_z^1, \boxtimes) \rightarrow (\mathcal{MD}, \cdot)$ since we can view A_z as a subset of A_z^{bi} . To define the stuffle brackets $[s_1, \dots, s_l]^*$, which fulfill the stuffle product, we use the above proposition to deform the quasi-shuffle product \boxtimes of the brackets into the stuffle product $*$, i.e. we use the following compositions of maps to get a algebra homomorphism from $(\mathfrak{H}_z^1, *)$ to \mathcal{MD} .

$$\begin{array}{ccc} (\mathfrak{H}_z^1, *) & \xrightarrow{[\dots]^*} & (\mathcal{MD}, \cdot) \\ \log_* \downarrow & & \uparrow [\dots] \\ (\mathfrak{H}_z^1, \sqcup) & \xrightarrow{\exp_{\boxtimes}} & (\mathfrak{H}_z^1, \boxtimes) \end{array}$$

Definition 5.2. Define for $s_1, \dots, s_l \in \mathbb{N}$ the *stuffle bracket* $[s_1, \dots, s_l]^*$ as the image of $z_{s_1} \dots z_{s_l}$ under the above map, i.e

$$[s_1, \dots, s_l]^* = [\exp_{\boxtimes}(\log_*(z_{s_1} \dots z_{s_l}))].$$

By \mathcal{MD}^* (resp. qMZ^*) we denote the spaces spanned by all (resp. all with $s_1 \geq 1$) stuffle brackets and 1.

Remember that the quasi-shuffle product \boxtimes for brackets was induced by the following map on $\mathbb{Q}A$

$$z_{s_1} \boxtimes z_{s_2} = \sum_{j=1}^{s_1} \lambda_{s_1, s_2}^j z_j + \sum_{j=1}^{s_2} \lambda_{s_2, s_1}^j z_j + z_{s_1+s_2} =: z_{s_1+s_2} + \sum_{j \geq 1} \gamma_{s_1, s_2}^j z_j,$$

where we define the γ_{s_1, s_2}^j just for simplicity of the following formulas. Since $\log_*(z_{s_1} z_{s_2}) = z_{s_1} z_{s_2} - \frac{1}{2} z_{s_1+s_2}$ and $\exp_{\boxtimes}(z_{s_1} z_{s_2}) = z_{s_1} z_{s_2} + \frac{1}{2} z_{s_1+s_2} + \frac{1}{2} \sum_j \gamma_{s_1, s_2}^j z_j$ we obtain $\exp_{\boxtimes}(\log_*(z_{s_1} z_{s_2})) = z_{s_1} z_{s_2} + \frac{1}{2} \sum_j \gamma_{s_1, s_2}^j z_j$, i.e.

$$[s_1, s_2]^* = [s_1, s_2] + \frac{1}{2} \sum_{j=1}^{s_1} \lambda_{s_1, s_2}^j [j] + \frac{1}{2} \sum_{j=1}^{s_2} \lambda_{s_2, s_1}^j [j].$$

Similarly one computes the length three case and obtains

$$\begin{aligned} [s_1, s_2, s_3]^* &= [s_1, s_2, s_3] + \frac{1}{2} \sum_{j \geq 0} \gamma_{s_1, s_2}^j [j, s_3] + \frac{1}{2} \sum_{j \geq 0} \gamma_{s_2, s_3}^j [s_1, j] - \frac{1}{12} \sum_{j \geq 0} \gamma_{s_1+s_2, s_3}^j [j] \\ &\quad - \frac{1}{4} \sum_{j \geq 0} \gamma_{s_1, s_2+s_3}^j [j] + \frac{1}{6} \sum_{j \geq 0} \gamma_{s_1, s_2}^j [j + s_3] + \frac{1}{6} \sum_{j_1, j_2 \geq 0} \gamma_{s_1, s_2}^{j_1} \gamma_{s_3, j_1}^{j_2} [j_2]. \end{aligned}$$

Example 5.3. For example we have $[1] \cdot [2, 1]^* = [1, 2, 1]^* + 2[2, 1, 1]^* + [3, 1]^* + [2, 2]^*$ with

$$\begin{aligned} [2, 1]^* &= [2, 1] - \frac{1}{4}[2], \quad [3, 1]^* = [3, 1] + \frac{1}{24}[2] - \frac{1}{4}[3], \quad [2, 2]^* = [2, 2] - \frac{1}{12}[2], \\ [2, 1, 1]^* &= [2, 1, 1] - \frac{3}{4}[2, 1] + \frac{11}{144}[2] - \frac{1}{24}[3], \\ [1, 2, 1]^* &= [1, 2, 1] - \frac{1}{4}[1, 2] - \frac{1}{4}[2, 1] + \frac{1}{72}[2] + \frac{1}{12}[3]. \end{aligned}$$

By construction we have the following

Proposition 5.4. Up to lower weight the stuffle brackets equal the brackets and therefore

$$\dim \left(\text{gr}_k^W(\mathfrak{qM}\mathcal{Z}) \right) = \dim \left(\text{gr}_k^W(\mathfrak{qM}\mathcal{Z}^*) \right).$$

Proof. This follows directly from the fact that \boxtimes and $*$ on \mathfrak{H}_z^1 are equal up to lower weights. \square

In Remark 6.6 we will see that the stuffle brackets can be used to define stuffle regularized multiple Eisenstein series. However as we will see, even though this version is easy to write down, this will not yield the "best" definition and we will use a more complicated construction.

We now want to define a q -series which is an element in \mathcal{BD} and which fulfills the "real" shuffle product of multiple zeta values. For $e_1, \dots, e_l \geq 1$ we generalize the generating function of bi-brackets to the following

$$\left| \begin{array}{c} X_1, \dots, X_l \\ Y_1, \dots, Y_l \\ e_1, \dots, e_l \end{array} \right| = \sum_{u_1 > \dots > u_l > 0} \prod_{j=1}^l E_{u_j}(Y_j) L_{u_j}(X_j)^{e_j}. \quad (5.1)$$

So in particular for $e_1 = \dots = e_l = 1$ these are the generating functions of the bi-brackets. To show that the coefficients of these series are in \mathcal{BD} for arbitrary e_j we need to define the differential operator $\mathcal{D}_{e_1, \dots, e_l}^Y := D_{Y_1, e_1} D_{Y_2, e_2} \dots D_{Y_l, e_l}$ with

$$D_{Y_j, e} = \prod_{k=1}^{e-1} \left(\frac{1}{k} \left(\frac{\partial}{\partial Y_{l-j+1}} - \frac{\partial}{\partial Y_{l-j+2}} \right) - 1 \right).$$

where we set $\frac{\partial}{\partial Y_{l+1}} = 0$.

Proposition 5.5. The coefficients of (5.1) are in \mathcal{BD} and it is

$$\mathcal{D}_{e_1, \dots, e_l}^Y \left| \begin{array}{c} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{array} \right| = \left| \begin{array}{c} Y_1 + \dots + Y_l, \dots, Y_1 \\ X_l, X_{l-1} - X_l, \dots, X_1 - X_2 \\ e_1, \dots, e_l \end{array} \right|.$$

Proof. By $\frac{\partial}{\partial X} L_n(X) = L_n(X)^2 + L_n(X)$ one inductively obtains

$$L_n(Y)^{e+1} = \left(\frac{1}{e} \frac{\partial}{\partial Y} - 1 \right) L_n(Y)^e = \prod_{k=1}^{e-1} \left(\frac{1}{k} \frac{\partial}{\partial Y} - 1 \right) L_n(Y),$$

from which the statement follows after a suitable change of variables. \square

Notice that in the case $e_1 = \dots = e_l = 1$ this is exactly the partition relation. We now want to define the shuffle brackets $[s_1, \dots, s_l]^\sqcup$ by using the following well-known fact :

Lemma 5.6. Let \mathcal{A} be an algebra spanned by elements a_{s_1, \dots, s_l} with $s_1, \dots, s_l \in \mathbb{N}$, let $H(X_1, \dots, X_l) = \sum_{s_j} a_{s_1, \dots, s_l} X_1^{s_1-1} \dots X_l^{s_l-1}$ be the generating functions of these elements and define for $f \in \mathbb{Q}[[X_1, \dots, X_l]]$

$$f^\sharp(X_1, \dots, X_l) = f(X_1 + \dots + X_l, X_2 + \dots + X_l, \dots, X_l).$$

Then the following two statements are equivalent

- i) The map $(\mathfrak{S}_{xy}^1, \sqcup) \rightarrow \mathcal{A}$ given by $z_{s_1} \dots z_{s_j} \mapsto a_{s_1, \dots, s_l}$ is an algebra homomorphism.
- ii) For all $r, s \in \mathbb{N}$ it is

$$H^\sharp(X_1, \dots, X_r) \cdot H^\sharp(X_{r+1}, \dots, X_{r+s}) = H^\sharp(X_1, \dots, X_{r+s})|_{sh_r^{(r+s)}},$$

where $sh_r^{(r+s)} = \sum_{\sigma \in \Sigma(r,s)} \sigma$ in the group ring $\mathbb{Z}[\mathfrak{S}_{r+s}]$ and the symmetric group \mathfrak{S}_r acts on $\mathbb{Q}[[X_1, \dots, X_r]]$ by $(f|\sigma)(X_1, \dots, X_r) = f(X_{\sigma^{-1}(1)}, \dots, X_{\sigma^{-1}(r)})$.

Proof. This can be proven by induction over l together with Proposition 8 in [I]. \square

Theorem 5.7. For $s_1, \dots, s_l \in \mathbb{N}$ define $[s_1, \dots, s_l]^{\sqcup} \in \mathcal{BD}$ as the coefficients of the following generating function

$$\begin{aligned} H_{\sqcup}(X_1, \dots, X_l) &= \sum_{s_1, \dots, s_l \geq 1} [s_1, \dots, s_l]^{\sqcup} X_1^{s_1-1} \dots X_l^{s_l-1} \\ &:= \sum_{\substack{1 \leq m \leq l \\ i_1 + \dots + i_m = l}} \frac{1}{i_1! \dots i_m!} \mathcal{D}_{i_1, \dots, i_m}^Y \left| \begin{array}{c} X_1, X_{i_m+1}, X_{i_{m-1}+i_m+1}, \dots, X_{i_2+\dots+i_m+1} \\ Y_1, \dots, Y_l \end{array} \right|_{Y=0}. \end{aligned}$$

Then we have the following two statements

i) The $[s_1, \dots, s_l]^{\sqcup}$ fulfill the shuffle product, i.e.

$$H_{\sqcup}^{\sharp}(X_1, \dots, X_r) \cdot H_{\sqcup}^{\sharp}(X_{r+1}, \dots, X_{r+s}) = H_{\sqcup}^{\sharp}(X_1, \dots, X_{r+s})_{|sh_r^{(r+s)}}.$$

ii) For $s_1 \geq 1, s_2, \dots, s_l \geq 2$ we have $[s_1, \dots, s_l]^{\sqcup} = [s_1, \dots, s_l]$.

Proof. The first part of the proof is basically the same as in the discussion in section 4.1 in [BT] but with a reverse order and some changes in the notation. Consider the alphabet $A = \left\{ \binom{y}{n} \mid n \in \mathbb{N}, y \in Y_{\mathbb{Z}} \right\}$, where $Y_{\mathbb{Z}}$ is the set of finite sums of the elements in $Y = \{Y_1, Y_2, \dots\}$. We denote a word in these letters by $\binom{y_1, \dots, y_l}{n_1, \dots, n_l}$. For two letters $a, b \in A$ define $a \diamond b \in A$ as the component-wise sum. With this we can equip $\mathbb{Q}\langle A \rangle$ with the quasi-shuffle product \odot (3.1) and therefore obtain a quasi-shuffle algebra $(\mathbb{Q}\langle A \rangle, \odot)$. It is easy to see that the map $(\mathbb{Q}\langle A \rangle, \odot) \rightarrow \mathcal{BD}_{\text{gen}}$ given by

$$\binom{y_1, \dots, y_l}{n_1, \dots, n_l} \mapsto \left| \begin{array}{c} 0, \dots, 0 \\ y_1, \dots, y_l \\ n_1, \dots, n_r \end{array} \right|$$

is an algebra homomorphism. Using now Proposition 5.1 the series h defined by the exponential map

$$h(X_1, \dots, X_r) = \sum_{\substack{1 \leq m \leq n \\ i_1 + \dots + i_m = n}} \frac{1}{i_1! \dots i_m!} \left| \begin{array}{c} 0, \dots, 0 \\ Y_1, \dots, Y_m \\ i_1, \dots, i_m \end{array} \right|,$$

where $Y_j = X_{i_1+\dots+i_{j-1}} + \dots + X_{i_1+\dots+i_j}$ with $X_0 := 0$, fulfills the (index-)shuffle product i.e.

$$h(X_1, \dots, X_r) \cdot h(X_{r+1}, \dots, X_{r+s}) = h(X_1, \dots, X_{r+s})_{|sh_r^{(r+s)}}.$$

We now set $H_{\sqcup}(X_1, \dots, X_l) := h(X_l, X_{l-1} - X_l, \dots, X_1 - X_2)$ and by the same argument as in Theorem 4.3 in [BT] it is

$$H_{\sqcup}^{\sharp}(X_1, \dots, X_r) \cdot H_{\sqcup}^{\sharp}(X_{r+1}, \dots, X_{r+s}) = H_{\sqcup}^{\sharp}(X_1, \dots, X_{r+s})_{|sh_r^{(r+s)}}.$$

Combining the definition of h and H_{\sqcup} we observe that $H_{\sqcup}(X_1, \dots, X_r)$ equals

$$\sum_{\substack{1 \leq m \leq n \\ i_1 + \dots + i_m = n}} \frac{1}{i_1! \dots i_m!} \left| \begin{array}{c} 0, \dots, 0 \\ X_{r-i_1+1}, X_{r-i_1-i_2+1} - X_{r-i_1+1}, \dots, X_1 - X_{r-i_1-\dots-i_{m-1}+1} \\ i_1, \dots, i_m \end{array} \right|.$$

We now apply Proposition 5.5 to this and obtain i) of the Theorem. To prove ii) one checks that the only summand on the right hand side, where **all** variables X_2, \dots, X_l appear, is the one with $i_1 = \dots = i_m = 1$ which is exactly $[s_1, \dots, s_l]X^{s_1-1} \dots X_l^{s_l-1}$. Therefore the shuffle bracket $[s_1, \dots, s_l]^{\sqcup}$ where $s_2, \dots, s_l \geq 2$ is given by the bracket $[s_1, \dots, s_l]$. \square

For low length we obtain the following examples:

Corollary 5.8. *It is $[s_1]^{\sqcup} = [s_1]$ and for $l = 2, 3, 4$ the $[s_1, \dots, s_l]^{\sqcup}$ are given by*

$$\begin{aligned}
i) \quad [s_1, s_2]^{\sqcup} &= [s_1, s_2] + \delta_{s_2,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1 \\ 1 \end{bmatrix} - [s_1] \right), \\
ii) \quad [s_1, s_2, s_3]^{\sqcup} &= [s_1, s_2, s_3] + \delta_{s_3,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_2 \\ 0, 1 \end{bmatrix} - [s_1, s_2] \right) \\
&\quad + \delta_{s_2,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_3 \\ 1, 0 \end{bmatrix} - \begin{bmatrix} s_1, s_3 \\ 0, 1 \end{bmatrix} - [s_1, s_3] \right) \\
&\quad + \delta_{s_2 \cdot s_3, 1} \cdot \frac{1}{6} \left(\begin{bmatrix} s_1 \\ 2 \end{bmatrix} - \frac{3}{2} \begin{bmatrix} s_1 \\ 1 \end{bmatrix} + [s_1] \right), \\
iii) \quad [s_1, s_2, s_3, s_4]^{\sqcup} &= [s_1, s_2, s_3, s_4] + \delta_{s_4,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_2, s_3 \\ 0, 0, 1 \end{bmatrix} - [s_1, s_2, s_3] \right) \\
&\quad + \delta_{s_3,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_2, s_4 \\ 0, 1, 0 \end{bmatrix} - \begin{bmatrix} s_1, s_2, s_4 \\ 0, 0, 1 \end{bmatrix} + [s_1, s_2, s_4] \right) \\
&\quad + \delta_{s_2,1} \cdot \frac{1}{2} \left(\begin{bmatrix} s_1, s_3, s_4 \\ 1, 0, 0 \end{bmatrix} - \begin{bmatrix} s_1, s_3, s_4 \\ 0, 1, 0 \end{bmatrix} + [s_1, s_3, s_4] \right) \\
&\quad + \delta_{s_2 \cdot s_4, 1} \cdot \frac{1}{4} \left(\begin{bmatrix} s_1, s_3 \\ 1, 1 \end{bmatrix} - 2 \begin{bmatrix} s_1, s_3 \\ 0, 2 \end{bmatrix} - \begin{bmatrix} s_1, s_3 \\ 1, 0 \end{bmatrix} + [s_1, s_3] \right) \\
&\quad + \delta_{s_3 \cdot s_4, 1} \cdot \frac{1}{6} \left(\begin{bmatrix} s_1, s_2 \\ 0, 2 \end{bmatrix} - \frac{3}{2} \begin{bmatrix} s_1, s_2 \\ 0, 1 \end{bmatrix} + [s_1, s_2] \right) \\
&\quad + \delta_{s_2 \cdot s_3, 1} \cdot \frac{1}{6} \left(\begin{bmatrix} s_1, s_4 \\ 0, 2 \end{bmatrix} - \begin{bmatrix} s_1, s_4 \\ 1, 1 \end{bmatrix} + \frac{3}{2} \begin{bmatrix} s_1, s_4 \\ 0, 1 \end{bmatrix} + \begin{bmatrix} s_1, s_4 \\ 2, 0 \end{bmatrix} - \frac{3}{2} \begin{bmatrix} s_1, s_4 \\ 1, 0 \end{bmatrix} + [s_1, s_4] \right) \\
&\quad + \delta_{s_2 \cdot s_3 \cdot s_4, 1} \cdot \frac{1}{24} \left(\begin{bmatrix} s_1 \\ 3 \end{bmatrix} - 2 \begin{bmatrix} s_1 \\ 2 \end{bmatrix} + \frac{11}{6} \begin{bmatrix} s_1 \\ 1 \end{bmatrix} - [s_1] \right).
\end{aligned}$$

Proof. This follows by calculating the coefficients of the series G_{\sqcup} in Theorem 5.7. \square

Proposition 5.9. For all $s_1, s_2 \geq 1$ it is

$$\begin{bmatrix} s_1, s_2 \\ 1, 0 \end{bmatrix}, \begin{bmatrix} s_1, s_2 \\ 0, 1 \end{bmatrix} \in \text{Fil}_{s_1+s_2+1,3}^{\text{W,L}}(\mathcal{MD})$$

Proof. First notice that from $\begin{bmatrix} s_1, s_2 \\ 1, 0 \end{bmatrix} \in \mathcal{MD}$ by the stuffle product for bi-brackets $\begin{bmatrix} s_1 \\ 1 \end{bmatrix} \cdot [s_2]$ one deduces $\begin{bmatrix} s_2, s_1 \\ 0, 1 \end{bmatrix} \in \mathcal{MD}$. Since the shuffle brackets fulfill the shuffle product we have

$$[s_1, s_2]^{\sqcup} \cdot [1] = 2[s_1, s_2, 1]^{\sqcup} + 2[s_1, 1, s_2]^{\sqcup} + 2[1, s_1, s_2]^{\sqcup} + \sum_{a,b,c \geq 2} \nu_{a,b,c} [a, b, c]^{\sqcup}$$

for some $\nu_{a,b,c} \in \mathbb{Q}$. By Proposition 5.8 the brackets $[s_1, s_2]^{\sqcup}$, $[1, s_1, s_2]^{\sqcup}$ and $[a, b, c]^{\sqcup}$ with $a, b, c \geq 2$ are elements of \mathcal{MD} , i.e. $2[s_1, s_2, 1]^{\sqcup} + 2[s_1, 1, s_2]^{\sqcup} \in \mathcal{MD}$. Using the explicit formula for the length three shuffle brackets it is easy to check that

$$2[s_1, s_2, 1]^{\sqcup} + 2[s_1, 1, s_2]^{\sqcup} = \begin{cases} \begin{bmatrix} s_1, s_2 \\ 1, 0 \end{bmatrix}, & s_2 > 1, \\ 2\begin{bmatrix} s_1, 1 \\ 0, 1 \end{bmatrix}, & s_2 = 1. \end{cases} \quad \text{mod } \mathcal{MD},$$

which proves the statement. \square

Finally we give some numerical results on the dimension of the space spanned by the shuffle brackets $[s_1, \dots, s_l]^{\sqcup}$. Denote by \mathcal{MD}^{\sqcup} the \mathbb{Q} -vector space spanned by all $[s_1, \dots, s_l]^{\sqcup}$ and 1 and $q\mathcal{MZ}^{\sqcup}$ spanned by those where $s_1 > 1$. By the use of the computer the author was able to give lower bounds for the dimension of $\text{gr}_k^{\text{W}}(\mathcal{MD}^{\sqcup})$ for $k \leq 10$ by using a fast implementation of the bi-brackets in Pari GP

k	0	1	2	3	4	5	6	7	8	9	10
$\dim(\text{gr}_k^{\text{W}}(q\mathcal{MZ}^{\sqcup})) \geq$	1	0	1	2	3	6	10	18	32	56	100

Table 1: Lower bounds for $\dim(\text{gr}_k^{\text{W}}(q\mathcal{MZ}^{\sqcup}))$.

We observe that these numbers coincide with the conjectured dimension for $\text{gr}_k^{\text{W}}(q\mathcal{MZ})$ given in [BK].

Remark 5.10. In the case of multiple zeta values the shuffle product is an easy consequence of the expression as an iterated integral. It is therefore a natural question whether there is also some kind of iterated integral expression from which the shuffle product follows. This was done for other q -analogue models of MZV in [Zh] and [MMEF] by the use of iterated Jackson integrals.

6 Multiple Eisenstein series G , G^{\sqcup} and G^*

In [BT] the authors defined regularized multiple Eisenstein series via the use of the coproduct structure on the space of formal iterated integrals. We will recall the basic facts in the following. It is important to notice that in [BT] the authors used a different order of the indices for multiple zeta values and multiple Eisenstein series. Here we will use the original order as in the paper [GKZ] and work [Ba].

Definition 6.1. For integers $s_1 \geq 3$ and $s_2, \dots, s_l \geq 2$, we define the *multiple Eisenstein series* $G_{s_1, \dots, s_l}(\tau)$ on \mathbb{H} by

$$G_{s_1, \dots, s_l}(\tau) = \sum_{\substack{\lambda_1 \succ \dots \succ \lambda_l \succ 0 \\ \lambda_i \in \Lambda_\tau}} \frac{1}{\lambda_1^{s_1} \dots \lambda_l^{s_l}},$$

where $\lambda_i \in \mathbb{Z}\tau + \mathbb{Z}$ are lattice points and the order \succ on $\mathbb{Z}\tau + \mathbb{Z}$ is given by

$$m_1\tau + n_1 \succ m_2\tau + n_2 \Leftrightarrow (m_1 > m_2 \vee (m_1 = m_2 \wedge n_1 > n_2)).$$

Remark 6.2. It is easy to see that these are holomorphic functions in the upper half plane and that they fulfill the stuffle product, i.e. it is for example

$$G_3(\tau) \cdot G_4(\tau) = G_{3,4}(\tau) + G_{4,3}(\tau) + G_7(\tau).$$

The condition $s_1 \geq 3$ is necessary for absolutely convergence of the sum. By choosing a specific way of summation we can also restrict this condition to get a definition of $G_{s_1, \dots, s_l}(\tau)$ with $s_1 = 2$ which also satisfies the stuffle product (see [BT] Definition 2.1).

Recall that we denote by $\mathcal{MZB} \subset \mathbb{C}[[q]]$ the space spanned by all q -series given by products of MZV, powers of $(-2\pi i)$ and bi-brackets. In [Ba] the Fourier expansion of multiple Eisenstein series was calculated. In particular the results in [Ba] show that we can consider G_{s_1, \dots, s_l} to be an element in \mathcal{MZB} by setting $q = e^{2\pi i\tau}$. For example

$$G_{3,2}(\tau) = \zeta(3, 2) + 3\zeta(3)g_2(q) + 2\zeta(2)g_3(q) + g_{3,2}(q) \in \mathcal{MZB},$$

where for all $s_1, \dots, s_l \geq 1$ we write $g_{s_1, \dots, s_l}(q) = (-2\pi i)^{s_1 + \dots + s_l} [s_1, \dots, s_l]$. We will also use the following notation

$$\begin{aligned} g_{s_1, \dots, s_l}^{\sqcup}(q) &= (-2\pi i)^{s_1 + \dots + s_l} [s_1, \dots, s_l]^{\sqcup}, \\ g_{\substack{s_1, \dots, s_l \\ r_1, \dots, r_l}}(q) &= (-2\pi i)^{s_1 + r_1 + \dots + s_l + r_l} \left[\begin{matrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{matrix} \right]. \end{aligned}$$

Later we will suppress the dependence of q and τ and just write g_{s_1, \dots, s_l} instead of $g_{s_1, \dots, s_l}(q)$ and similar for the other functions considered above.

Following Goncharov ([G]) the authors in [BT] consider the algebra \mathcal{I} generated by the elements $\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1})$, where $a_i \in \{0, 1\}$, $N \geq 0$, with the product given by the shuffle product \sqcup together with relations coming from real iterated integrals (see [G] Section 2 and [BT] Section 3 for details but with a different order). This space has the structure of a Hopf algebra with the coproduct given by

$$\begin{aligned} \Delta_G(\mathbb{I}(a_0; a_1, \dots, a_N; a_{N+1})) &:= \\ \sum \left(\mathbb{I}(a_0; a_{i_1}, \dots, a_{i_k}; a_{N+1}) \otimes \prod_{p=0}^k \mathbb{I}(a_{i_p}; a_{i_p+1}, \dots, a_{i_{p+1}-1}; a_{i_{p+1}}) \right), \end{aligned} \quad (6.1)$$

where the sum runs over all $i_0 = 0 < i_1 < \dots < i_k < i_{k+1} = N + 1$ with $0 \leq k \leq N$. The triple $(\mathcal{I}, \sqcup, \Delta_G)$ is a commutative graded Hopf algebra over \mathbb{Q} ([G] Proposition 2.2). For integers $n \geq 0, s_1, \dots, s_r \geq 1$, we set

$$I_n(s_1, \dots, s_r) := I(1; \underbrace{0, 0, \dots, 1}_{s_1}, \dots, \underbrace{0, 0, \dots, 1}_{s_r}, \underbrace{0, \dots, 0}_n; 1).$$

In particular, we write $I(s_1, \dots, s_r)$ to denote $I_0(s_1, \dots, s_r)$. The quotient space $\mathcal{I}^1 = \mathcal{I}/\mathbb{I}(0; 0; 1)\mathcal{I}$ also has the structure of a Hopf algebra with the same coproduct and due to Proposition 3.2 in [BT] the elements $I(s_1, \dots, s_l)$ form a basis of \mathcal{I}^1 , i.e. as a \mathbb{Q} -algebra the space \mathcal{I}^1 is isomorphic to $(\mathfrak{H}_{xy}^1, \sqcup)$ by sending $I(s_1, \dots, s_l)$ to $z_{s_1} \dots z_{s_l}$. In the following we therefore consider \mathfrak{H}_{xy}^1 as a Hopf algebra with the above coproduct.

Proposition 6.3. [IKZ](shuffle & stuffle regularized MZV) There exist algebra homomorphisms $Z^\sqcup : (\mathfrak{H}_{xy}^1, \sqcup) \rightarrow \mathcal{MZ}$ and $Z^* : (\mathfrak{H}_z^1, *) \rightarrow \mathcal{MZ}$ with $\zeta^\sqcup(s_1, \dots, s_l) = Z^\sqcup(z_{s_1} \dots z_{s_l})$ and $\zeta(s_1, \dots, s_l)^* = Z^\sqcup(z_{s_1} \dots z_{s_l})$ such that

$$\zeta^*(s_1, \dots, s_l) = \zeta^\sqcup(s_1, \dots, s_l) = \zeta(s_1, \dots, s_l)$$

for $s_l \geq 2$ and $s_2, \dots, s_l \geq 1$. They are uniquely determined by $Z^\sqcup(z_1) = Z^*(z_1) = 0$.

Proof. This follows from the results of section 2 in [IKZ]. \square

We now recall the definition of G^\sqcup from [BT].

Definition 6.4. For integers $s_1, \dots, s_l \geq 1$, define the q -series $G_{s_1, \dots, s_l}^\sqcup(q) \in \mathcal{MZB}$, called (*shuffle*) *regularized multiple Eisenstein series*, as

$$G_{s_1, \dots, s_l}^\sqcup(q) := m((\mathfrak{g}^\sqcup \otimes Z^\sqcup) \circ \Delta_G(z_{s_1} \dots z_{s_l})),$$

where $\mathfrak{g}^\sqcup : (\mathfrak{H}_{xy}^1, \sqcup) \rightarrow \mathbb{C}[[q]]$ is the algebra homomorphism defined by $\mathfrak{g}^\sqcup(z_{s_1} \dots z_{s_l}) = g_{s_1, \dots, s_l}^\sqcup(q)$ and m denotes the multiplication given by $m : a \otimes b \mapsto a \cdot b$.

We can view G^\sqcup as an algebra homomorphism $G^\sqcup : (\mathfrak{H}_{xy}^1, \sqcup) \rightarrow \mathcal{MZB}$ such that the following diagram commutes

$$\begin{array}{ccc} (\mathfrak{H}_{xy}^1, \sqcup) & \xrightarrow{\Delta_G} & (\mathfrak{H}_{xy}^1, \sqcup) \otimes (\mathfrak{H}_{xy}^1, \sqcup) \\ G^\sqcup \downarrow & & \downarrow Z^\sqcup \otimes \mathfrak{g}^\sqcup \\ \mathcal{MZB} & \xleftarrow{m} & \mathcal{MZ} \otimes \mathbb{C}[[q]] \end{array}$$

Summarizing the results of [BT] we have

Theorem 6.5. [BT] For all $s_1, \dots, s_l \geq 1$ and $q = e^{2\pi i\tau}$ with $\tau \in \mathbb{H}$ the regularized multiple Eisenstein series $G_{s_1, \dots, s_l}^\sqcup(q)$ have the following properties:

- i) They are holomorphic functions on the upper half plane having a Fourier expansion with the regularized multiple zeta values as the constant term.

-
- ii) They fulfill the shuffle product, i.e. we have an algebra homomorphism $(\mathfrak{H}_{xy}^1, \sqcup) \rightarrow \mathcal{MZB}$ by sending the generators $z_{s_1} \dots z_{s_l}$ to $G_{s_1, \dots, s_l}^{\sqcup}(q)$.
- iii) For integers $s_1, \dots, s_l \geq 2$ they equal the multiple Eisenstein series

$$G_{s_1, \dots, s_l}^{\sqcup}(q) = G_{s_1, \dots, s_l}(q)$$

and therefore they fulfill the stuffle product (see Remark 6.2) in these cases.

Theorem 6.5 provides a large family of linear relations between the G^{\sqcup} , since one can write the product $G_{s_1, \dots, s_l}^{\sqcup}(q) \cdot G_{r_1, \dots, r_m}^{\sqcup}(q)$ in two different ways whenever one has $s_1, \dots, s_l, r_1, \dots, r_m \geq 2$ by using the stuffle and shuffle product formula. We will call these relations the restricted double shuffle relations, since they are just a subset of all (finite) double shuffle relations of MZV, where the indices s_j and r_i are additionally allowed to be 1 whenever $j < l$ and $i < m$. We compare the number of both relations at the end of this paper.

Numerical experiments suggest (see the dimension discussion at the end of [BT]), that there are additional relations between the G^{\sqcup} coming from the double shuffle relations, where some indices are also allowed to be 1. It is therefore interesting to understand the exact failure of the stuffle product for the regularized multiple Eisenstein G^{\sqcup} which seems not to be covered best possible by the Theorem 6.5. In the following we want to sketch a possible approach to answer this question. The basic idea is to define stuffle regularized multiple Eisenstein series G_{s_1, \dots, s_l}^* which equals the shuffle regularized ones in most of the cases. For this we need the following: For an arbitrary quasi-shuffle algebra $\mathbb{Q}\langle A \rangle$ define on the following coproduct for a word w

$$\Delta_H(w) = \sum_{uv=w} u \otimes v.$$

Then it is known due to Hoffman ([H]) that the space $(\mathbb{Q}\langle A \rangle, \odot, \Delta_H)$ has the structure of a bialgebra. With this we try to mimic the definition of the G^{\sqcup} and use the coproduct structure on the space $(\mathfrak{H}_z^1, *, \Delta_H)$ to define G^* , i.e. we consider the following diagram

$$\begin{array}{ccc} (\mathfrak{H}_z^1, *) & \xrightarrow{\Delta_H} & (\mathfrak{H}_z^1, *) \otimes (\mathfrak{H}_z^1, *) \\ G^* \downarrow & & \downarrow \mathfrak{g}^* \otimes Z^* \\ \mathbb{C}[[q]] & \xleftarrow{m} & \mathbb{C}[[q]] \otimes \mathcal{MZ} \end{array}$$

with a suitable choice of an algebra homomorphism $\mathfrak{g}^* : (\mathfrak{H}_z^1, *) \rightarrow \mathbb{C}[[q]]$.

Remark 6.6. One naive way to define \mathfrak{g}^* would be to define it on the generator $w = z_{s_1} \dots z_{s_l}$ by $(-2\pi i)^{s_1 + \dots + s_l} [s_1, \dots, s_l]^*$ which would yield stuffle regularized the multiple Eisenstein series which coincide with the G^{\sqcup} in the length one case. But already in length two this differs from the original multiple Eisenstein series even when all $s_j \geq 2$ for example it is

$$G_{3,2}(\tau) = G_{3,2}^{\sqcup}(\tau) = \zeta(3, 2) + 3\zeta(3)g_2(q) + 2\zeta(2)g_3(q) + g_{3,2}(q)$$

but the naive approach would give $\zeta(3, 2) + 2\zeta(2)g_3(q) + g_{2,3}(q)$. Even though these are similar this seems not to be the definition we want and we need to find an alternative definition for \mathfrak{g}^* in the following such that G^* coincide with the original multiple Eisenstein series.

Motivated by the calculation of the Fourier expansion of multiple Eisenstein series described in [Ba] and [BT] we consider the following construction.

Construction 6.7. Given a \mathbb{Q} -algebra (A, \cdot) and a family of homomorphism

$$\{w \mapsto f_w(m)\}_{m \in \mathbb{N}}$$

from $(\mathfrak{H}_z^1, *)$ to (A, \cdot) , we define for $w \in \mathfrak{H}_z^1$ and $M \in \mathbb{N}$

$$F_w(M) := \sum_{\substack{1 \leq k \leq l(w) \\ w_1 \dots w_k = w \\ M > m_1 > \dots > m_k > 0}} f_{w_1}(m_1) \dots f_{w_k}(m_k) \in A,$$

where $l(w)$ denotes the length of the word w and $w_1 \dots w_k = w$ is a decomposition of w into k words in \mathfrak{H}_z^1 .

Proposition 6.8. For all $M \in \mathbb{N}$ the map from $(\mathfrak{H}_z^1, *)$ to (A, \cdot) defined by $w \mapsto F_w(M)$ is an algebra homomorphism, i.e. $\{w \mapsto F_w(m)\}_{m \in \mathbb{N}}$ is again a family of homomorphism as in the Construction 6.7.

Proof. We use the coproduct structure on $(\mathfrak{H}_z^1, *, \Delta_H)$ to prove the statement by induction over M . It is $F_w(1) = 0$ which clearly fulfills the stuffle product. For the induction step one checks that $F_w(M+1) = \sum_{uv=w} F_u(M)f_v(M)$ which is exactly the image of w under $(F(M) \otimes f(M)) \circ \Delta_H$, i.e. it fulfills the stuffle product by the induction hypothesis. \square

For a word $w = z_{s_1} \dots z_{s_l} \in \mathfrak{H}^1$ we also write in the following $f_{s_1, \dots, s_l}(m) := f_w(m)$ and similarly $F_{s_1, \dots, s_l}(M) := F_w(M)$.

Example 6.9. Let $f_w(m)$ be as in the construction. In small lengths the F_w are given by

$$\begin{aligned} F_{s_1}(M) &= \sum_{M > m_1 > 0} f_{s_1}(m_1), \\ F_{s_1, s_2}(M) &= \sum_{M > m_1 > 0} f_{s_1, s_2}(m_1) + \sum_{M > m_1 > m_2 > 0} f_{s_1}(m_1) f_{s_2}(m_2) \end{aligned}$$

and one can check directly by the use of the stuffle product for the f_w that

$$\begin{aligned}
F_{s_1}(M) \cdot F_{s_2}(M) &= \sum_{M>m_1>0} f_{s_1}(m_1) \cdot \sum_{M>m_2>0} f_{s_2}(m_2) \\
&= \sum_{M>m_1>m_2>0} f_{s_1}(m_1)f_{s_2}(m_2) + \sum_{M>m_2>m_1>0} f_{s_2}(m_2)f_{s_1}(m_1) + \sum_{M>m_1>0} f_{s_1}(m_1)f_{s_2}(m_1) \\
&= \sum_{M>m_1>m_2>0} f_{s_1}(m_1)f_{s_2}(m_2) + \sum_{M>m_2>m_1>0} f_{s_2}(m_2)f_{s_1}(m_1) \\
&+ \sum_{M>m_1>0} (f_{s_1,s_2}(m_1) + f_{s_2,s_1}(m_1) + f_{s_1+s_2}(m_1)) \\
&= F_{s_1,s_2}(M) + F_{s_2,s_1}(M) + F_{s_1+s_2}(M).
\end{aligned}$$

Let us now give an explicit example for maps f_w in which we are interested. For this we need to define the following

Definition 6.10. For integers $s_1, \dots, s_l \geq 1$ with $s_1, s_l \geq 2$ we define a holomorphic function $\Psi_{s_1, \dots, s_l}(z)$ on $\mathbb{C} - \mathbb{Z}$ called the *multitangent function* by

$$\Psi_{s_1, \dots, s_l}(z) = \sum_{\substack{n_1 > \dots > n_l \\ n_j \in \mathbb{Z}}} \frac{1}{(z + n_1)^{s_1} \cdots (z + n_l)^{s_l}}.$$

When $l = 1$ we refer to $\Psi_{s_1}(z)$ as the *monotangent function*.

In [Bo] the author uses the notation $\mathcal{T}e^{n_1, \dots, n_r}(z)$ which corresponds to our $\Psi_{n_1, \dots, n_r}(z)$ and showed that the series defining $\Psi_{n_1, \dots, n_r}(z)$ converges absolutely when $n_1, \dots, n_r \geq 2$. These functions fulfill (for the cases they are defined) the stuffle product. The multitangent functions appear in the calculation of the Fourier expansion of the multiple Eisenstein series G_{s_1, \dots, s_l} (see [Ba], [BT]), for example in length two it is

$$G_{s_1, s_2}(\tau) = \zeta(s_1, s_2) + \zeta(s_1) \sum_{m_1 > 0} \Psi_{s_2}(m_1\tau) + \sum_{m_1 > 0} \Psi_{s_1, s_2}(m_1\tau) + \sum_{m_1 > m_2 > 0} \Psi_{s_1}(m_1\tau)\Psi_{s_2}(m_2\tau).$$

One nice result of [Bo] is a regularization of the multitangent function to get a definition of $\Psi_{s_1, \dots, s_l}(z)$ for all $s_1, \dots, s_l \in \mathbb{N}$. We will use this result together with the above construction to recover the Fourier expansion of the multiple Eisenstein series.

Theorem 6.11. ([Bo]) For all $s_1, \dots, s_l \in \mathbb{N}$ there exist holomorphic functions Ψ_{s_1, \dots, s_l} on \mathbb{H} with the following properties

- i) Setting $q = e^{2\pi i\tau}$ for $\tau \in \mathbb{H}$ the map $w \mapsto \Psi_w(\tau)$ defines an algebra homomorphism from $(\mathfrak{H}_z^1, *)$ to $(\mathbb{C}[[q]], \cdot)$.
- ii) In the case $s_1, s_l \geq 2$ the Ψ_{s_1, \dots, s_l} are given by the multitangent functions in Definition 6.10.
- iii) The monotangents functions have the q -expansion given by

$$\Psi_1(\tau) = \frac{\pi}{\tan(\pi\tau)} = (-2\pi i) \left(\frac{1}{2} + \sum_{n>0} q^n \right), \quad \Psi_k(\tau) = \frac{(-2\pi i)^k}{(k-1)!} \sum_{n>0} n^{k-1} q^n \text{ for } k \geq 2.$$

iv) (Reduction into monotangent function) Every $\Psi_{s_1, \dots, s_l}(\tau)$ can be written as a \mathcal{MZ} -linear combination of monotangent functions. There are explicit $\epsilon_{i,k}^{s_1, \dots, s_l} \in \mathcal{MZ}$ s.th.

$$\Psi_{s_1, \dots, s_l}(\tau) = \delta^{s_1, \dots, s_l} + \sum_{i=1}^l \sum_{k=1}^{s_i} \epsilon_{i,k}^{s_1, \dots, s_l} \Psi_k(\tau),$$

where $\delta^{s_1, \dots, s_l} = \frac{(\pi i)^l}{l!}$ if $s_1 = \dots = s_l = 1$ and l even and $\delta^{s_1, \dots, s_l} = 0$ otherwise. For $s_1 > 1$ and $s_l > 1$ the sum on the right starts at $k = 2$, i.e. there are no $\Psi_1(\tau)$ appearing and therefore there is no constant term in the q -expansion.

Proof. This is just a summary of the results in Section 6 and 7 of [Bo]. The last statement is given by Theorem 6 there. \square

Due to iv) in the Theorem the calculation of the Fourier expansion of multiple Eisenstein series, where ordered sums of multitangent functions appear, reduces to ordered sums of monotangent functions. The connection of these sums to the brackets, i.e. to the functions g , is given by the following fact which can be seen by using iii) of the above Theorem. For $n_1, \dots, n_r \geq 2$ it is

$$g_{s_1, \dots, s_r}(q) = \sum_{m_1 > \dots > m_l > 0} \Psi_{s_1}(m_1 \tau) \dots \Psi_{s_l}(m_l \tau).$$

For $w \in \mathfrak{H}_z^1$ we now use the Construction 6.7 with $A = \mathbb{C}[[q]]$ and the family of homomorphism $\{w \mapsto \Psi_w(n\tau)\}_{n \in \mathbb{N}}$ to define

$$\mathfrak{g}^{*,M}(w) := (-2\pi i)^{|w|} \sum_{\substack{1 \leq k \leq l(w) \\ w_1 \dots w_k = w}} \sum_{M > m_1 > \dots > m_k > 0} \Psi_{w_1}(m_1 \tau) \dots \Psi_{w_k}(m_k \tau).$$

From Proposition 6.8 and the Theorem 6.11 it follows that for all $M \in \mathbb{N}$ the map $\mathfrak{g}^{*,M}$ is an algebra homomorphism from $(\mathfrak{H}_z^1, *)$ to $\mathbb{C}[[q]]$.

Definition 6.12. For integers $s_1, \dots, s_l \geq 1$ and $M \in \mathbb{N}$, we define the q -series $G_{s_1, \dots, s_l}^{*,M}(q) \in \mathbb{C}[[q]]$ as the image of the word $w = z_{s_1} \dots z_{s_l} \in \mathfrak{H}_z^1$ under the algebra homomorphism $(Z^* \otimes \mathfrak{g}^{*,M}) \circ \Delta_H$:

$$G_{s_1, \dots, s_l}^{*,M}(\tau) := m \left((\mathfrak{g}^{*,M} \otimes Z^*) \circ \Delta_H(w) \right) \in \mathbb{C}[[q]].$$

For $s_1, \dots, s_l \geq 2$ it is easy to see that the limit

$$G_{s_1, \dots, s_l}^*(\tau) := \lim_{M \rightarrow \infty} G_{s_1, \dots, s_l}^{*,M}(\tau)$$

exists and that we have

Proposition 6.13. For $s_1, \dots, s_j \geq 2$ we have $G_{s_1, \dots, s_l} = G_{s_1, \dots, s_l}^* = G_{s_1, \dots, s_l}^{\sqcup}$.

Proof. This follows since the construction above was exactly the one which appears in the calculation of the Fourier expansion of multiple Eisenstein series. See [Ba] and [BT] for details. \square

We now want to discuss whether the limit of $G_{s_1, \dots, s_l}^{*,M}(\tau)$ as $M \rightarrow \infty$ exists for more general $s_1, \dots, s_l \in \mathbb{N}$. Since it is a finite sum of ordered sums of multitangent functions we can, by Theorem 6.11 iv), restrict to the case of ordered sums of monotangent functions and powers of π , i.e. we want to determine when the limit of

$$\sum_{M > m_1 > \dots > m_l > 0} f_1(m\tau) \dots f_l(m\tau)$$

with $f_j(\tau) = \Psi_s(\tau)$ for some $s \in \mathbb{N}$ or $f_j(\tau) = 1$ exists. One easily checks that this is exactly the case when $f_1(\tau)$ has no constant term, i.e. $f_1(\tau) \neq \Psi_1(\tau)$ and $f_1(\tau) \neq 1$. We deduce that therefore the limit of $G_{s_1, \dots, s_l}^{*,M}(\tau)$ as $M \rightarrow \infty$ exists when all $\Psi_{s_1, \dots, s_l}, \Psi_{s_1, \dots, s_{l-1}}, \dots, \Psi_{s_1}$ have no constant term. Even though the Theorem 6.11 iv) justifies this for the case all $s_j \geq 2$ we see, by using the explicit reductions to monotangents given in [Bo], that for low weights in fact the $\Psi_{1, \dots, 1}(\tau)$ are the only multitangent functions with constant term. This question remains open but seems to be crucial in order to get a definition of G^* for all admissible indices.

Remark 6.14. That $\Psi_{1, \dots, 1}(\tau)$ are the only multitangent functions with a constant term is also expected by the author of [Bo]. Since there is no proof of this statement so far, we just use this here in low length, where the explicit formulas for the Ψ are known.

The functions $g_{r_1, \dots, r_l}^{(s_1, \dots, s_l)}$, i.e. the bi-brackets, will appear in G_{s_1, \dots, s_l}^* every time there is a $j < l$ with $s_j = 1$ as we will see in the following examples:

Example 6.15. i) We are going to calculate $G_{2,1,2}^*$. For this we use the Table 1 and 6 at the end of [Bo] where one can find that $\Psi_{2,1,2}(z) = \Psi_{1,2}(z) = \Psi_{2,1}(z) = 0$, therefore it is

$$\begin{aligned} G_{2,1,2}^{*,M}(\tau) &= \zeta(2, 1, 2)^* + \sum_{0 < m_1 < M} \Psi_2(m_1\tau) \cdot \zeta(1, 2)^* + \sum_{M > m_1 > m_2 > 0} \Psi_2(m_1\tau) \Psi_1(m_2\tau) \cdot \zeta(2)^* \\ &+ \sum_{M > m_1 > m_2 > m_3 > 0} \Psi_2(m_1\tau) \Psi_1(m_2\tau) \Psi_2(m_3\tau). \end{aligned}$$

Taking the limit $M \rightarrow \infty$ and using the explicit forms of Ψ_k ($k \geq 1$), $\zeta(2, 1, 2)^* = \zeta(2, 1, 2)$, $\zeta(2)^* = \zeta(2)$ and $\zeta(1, 2)^* = -\zeta(2, 1) - \zeta(3) = -2\zeta(2, 1)$ we obtain

$$\begin{aligned} G_{2,1,2}^* &= \lim_{M \rightarrow \infty} G_{2,1,2}^{*,M} \\ &= \zeta(2, 1, 2) - 2\zeta(2, 1)g_2 + \zeta(2) \left(g_{2,1} + \frac{1}{2}g_{(1)}^{(2)} - \frac{(-2\pi i)}{2}g_2 \right) \\ &\quad + g_{2,1,2} + \frac{1}{2} \left(g_{(0,1)}^{(2,2)} - g_{(1,0)}^{(2,2)} - (-2\pi i)g_{2,2} \right) \\ &= \zeta(2, 1, 2) - 2\zeta(1, 2)g_2^{\sqcup\sqcup} + \zeta(2)g_{2,1}^{\sqcup\sqcup} + g_{2,1,2}^{\sqcup\sqcup} \\ &= G_{2,1,2}^{\sqcup\sqcup}. \end{aligned}$$

Similarly one can prove that $G_{2,1}^{\sqcup} = G_{2,1}^*$, $G_{2,2,1}^{\sqcup} = G_{2,2,1}^*$ and $G_{4,1}^{\sqcup} = G_{4,1}^*$ from which we obtain the following stuffle product in weight 5:

$$G_2^{\sqcup} \cdot G_{2,1}^{\sqcup} = G_{2,1,2}^{\sqcup} + 2G_{2,2,1}^{\sqcup} + G_{4,1}^{\sqcup} + G_{2,3}^{\sqcup}. \quad (6.2)$$

ii) There are G_{s_1, \dots, s_l}^* that differ from $G_{s_1, \dots, s_l}^{\sqcup}$. For example it is

$$\begin{aligned} G_{2,1,1}^* &= \zeta(2, 1, 1) - \frac{13}{2}\zeta(2)g_2 - (-2\pi i)g_{2,1} + \frac{1}{2}g_{(1,0)}^{(2,1)} - \frac{3}{8}(-2\pi i)g_{(1)}^{(2)} + \frac{1}{4}g_{(2)}^{(2)} + g_{2,1,1}, \\ G_{2,1,1}^{\sqcup} &= \zeta(2, 1, 1) - 4\zeta(2)g_2 - (-2\pi i)g_{2,1} + \frac{1}{2}g_{(1,0)}^{(2,1)} - \frac{3}{12}(-2\pi i)g_{(1)}^{(2)} + \frac{1}{6}g_{(2)}^{(2)} + g_{2,1,1}, \\ G_{2,1,1}^{\sqcup} - G_{2,1,1}^* &= \frac{5}{2}g_2 + \frac{1}{8}(-2\pi i)g_{(1)}^{(2)} - \frac{1}{12}g_{(2)}^{(2)} \neq 0 \end{aligned}$$

It is still an open question for which indices s_1, \dots, s_l we have $G_{s_1, \dots, s_l}^{\sqcup} = G_{s_1, \dots, s_l}^*$. The author wants to address this question in upcoming projects.

We end this paper by a comparison of different version of the double shuffle relations. For this we write for words $u, v \in \mathfrak{H}^1$, $ds(u, v) = u \sqcup v - u * v \in \mathfrak{H}^1$, where the \sqcup is again the shuffle product with respect to the alphabet $\{x, y\}$ and $*$ the stuffle product with respect to the alphabet $\{z_1, z_2, \dots\}$. Write \mathfrak{H}^0 for the algebra of all admissible words, i.e. $\mathfrak{H}^0 = 1 \cdot \mathbb{Q} + x\mathfrak{H}y$, and set $\mathfrak{H}^2 = \mathbb{Q}\langle\{z_2, z_3, \dots\}\rangle$ to be the span of all words in \mathfrak{H}^1 with no z_1 occurring, i.e. the words for which the multiple Eisenstein series G exists.

With this we define the numbers eds_k (extended double shuffle relations of weight k), fds_k (finite double shuffle relations of weight k) and rds_k (restricted finite double shuffle relations of weight k) by

$$\begin{aligned} eds_k &:= \dim_{\mathbb{Q}} \langle ds(u, v) \in \mathfrak{H}^1 \mid |u| + |v| = k, u \in \mathfrak{H}^0, v \in \mathfrak{H}^0 \cup \{y\} \rangle_{\mathbb{Q}}, \\ fds_k &:= \dim_{\mathbb{Q}} \langle ds(u, v) \in \mathfrak{H}^1 \mid |u| + |v| = k, u, v \in \mathfrak{H}^0 \rangle_{\mathbb{Q}}, \\ rds_k &:= \dim_{\mathbb{Q}} \langle ds(u, v) \in \mathfrak{H}^1 \mid |u| + |v| = k, u, v \in \mathfrak{H}^2 \rangle_{\mathbb{Q}}. \end{aligned}$$

For the number of admissible generators of weight k which equals 2^{k-2} for $k > 1$, i.e. words in \mathfrak{H}^0 , we write gen_k . By Theorem 6.5 we know that the number of relations between the G^{\sqcup} of weight k is at least rds_k . But these relations don't suffice to give all relations between (shuffle) regularized multiple Eisenstein series since some of the finite double shuffle relations which are not restricted are also fulfilled. The numbers d_k

$$\sum_{k \geq 0} d_k X^k = \frac{1}{1 - X^2 - X^3},$$

are the conjectured dimensions for \mathcal{MZ}_k . Since it is also conjectured that eds_k is the number of all relations between MZV of weight k one expects that $d_k = gen_k - eds_k$, which so far is not known. It was observed in [BT] that up to weight 7 the dimension of

$$\mathcal{E}_k = \langle G_{s_1, \dots, s_l}^{\sqcup}(q) \mid k = s_1 + \dots + s_l, l \geq 0, s_1, \dots, s_{l-1} \geq 1, s_l \geq 2 \rangle_{\mathbb{Q}}$$

seems to be the same as the dimension of $\text{gr}_k^W(\mathfrak{qMZ})$. The following table gives an overview of these numbers up to weight 14.

k	1	2	3	4	5	6	7	8	9	10	11	12	13	14
eds_k	0	0	1	3	6	14	29	60	123	249	503	1012	2032	4075
fds_k	0	0	0	1	2	7	16	40	92	200	429	902	1865	3832
rds_k	0	0	0	1	1	3	5	11	19	37	65	120	209	372
gen_k	0	1	2	4	8	16	32	64	128	256	512	1024	2048	4096
$d_k \stackrel{?}{=} gen_k - eds_k$	0	1	1	1	2	2	3	4	5	7	9	12	16	21
$\dim \mathcal{E}_k \geq$	0	1	2	3	6	10	18	?	?	?	?	?	?	?

Table 2: Comparison of the number of extended-, finite-, and restricted-double shuffle relations.

The last line give lower bounds of the dimension of the space \mathcal{E}_k spanned by all admissible shuffle regularized multiple Eisenstein series of weight k which are for $k \leq 5$ exact since we derived all relations up to this weight.

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E-mail:

henrik.bachmann@uni-hamburg.de

FACHBEREICH MATHEMATIK (AZ)

UNIVERSITÄT HAMBURG

BUNDESSTRASSE 55

D-20146 HAMBURG

Appendix D

A short note on a conjecture of Okounkov about a q -analogue of multiple zeta values

A short note on a conjecture of Okounkov about a q -analogue of multiple zeta values

HENRIK BACHMANN, ULF KÜHN

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Abstract

In [Ok] Okounkov studies a specific q -analogue of multiple zeta values and makes some conjectures on their algebraic structure. In this note we want to compare Okounkov's q -analogues to the generating function for multiple divisor sums defined in [BK].

1 Introduction

Multiple zeta values are natural generalizations of the Riemann zeta values that are defined for integers $s_1 > 1$ and $s_i \geq 1$ for $i > 1$ by

$$\zeta(s_1, \dots, s_l) := \sum_{n_1 > n_2 > \dots > n_l > 0} \frac{1}{n_1^{s_1} \dots n_l^{s_l}}.$$

Because of its occurrence in various fields of mathematics and physics these real numbers are of particular interest. In [Ok] Okounkov discusses a conjectural connection from enumerative geometry of some Hilbert schemes to a specific q -analogue $Z(s_1, \dots, s_l)$ of the multiple zeta-values. He denotes by \mathfrak{qMZV} the \mathbb{Q} -algebra generated by these. In this short note we want to discuss the connection of these q -multiple zeta values to the algebra \mathcal{MD} of generating functions for multiple divisor sums $[s_1, \dots, s_l]$ defined by the authors in [BK]. More precisely we have

Theorem 1.1. Let $\mathcal{MD}^\sharp = \langle [s_1, \dots, s_l] \in \mathcal{MD} \mid s_i > 1 \forall i \text{ or } s_1 = \emptyset \rangle_{\mathbb{Q}}$.

- i) The sub vector space \mathcal{MD}^\sharp is in fact a sub algebra of \mathcal{MD} .
- ii) We have $\mathfrak{qMZV} = \mathcal{MD}^\sharp$, in particular the \mathbb{Q} -vector space generated by the $Z(s_1, \dots, s_l)$ is closed under multiplication.

iii) We have $q \frac{d}{dq} Z(k) \in \mathfrak{qMZV}$ for all $k \geq 2$.

The first two statements are merely a reformulation results implicitly contained in [BK]. The third is direct consequence of some explicit formula given in [BK]. It gives some evidence to the conjecture of Okunkov, that the operator d is a derivation on \mathfrak{qMZV} .

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2 q -analogues of multiple zeta values

In the following we fix a subset $S \subset \mathbb{N}$, which we consider as the support for index entries, i.e. we assume $s_1, \dots, s_l \in S$. For each $s \in S$ we let $Q_s(t) \in \mathbb{Q}[t]$ be a polynomial with $Q_s(0) = 0$ and $Q_s(1) \neq 0$. We set $Q = \{Q_s(t)\}_{s \in S}$. A sum of the form

$$Z_Q(s_1, \dots, s_l) := \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{Q_{s_j}(q^{n_j})}{(1 - q^{n_j})^{s_j}} \quad (2.1)$$

with polynomials Q_s as before, defines a q -analogue of a multiple zeta-value of weight $k = s_1 + \dots + s_l$ and length l . Observe only because of $Q_{s_1}(0) = 0$ this defines an element of $\mathbb{Q}[[q]]$. This notion is due to the identity

$$\begin{aligned} \lim_{q \rightarrow 1} (1 - q)^k Z_Q(s_1, \dots, s_l) &= \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \lim_{q \rightarrow 1} \left(Q_{s_j}(q^{n_j}) \frac{(1 - q)^{s_j}}{(1 - q^{n_j})^{s_j}} \right) \\ &= Q_{s_1}(1) \dots Q_{s_l}(1) \cdot \zeta(s_1, \dots, s_l). \end{aligned}$$

Here we used that $\lim_{q \rightarrow 1} (1 - q)^s / (1 - q^n)^s = 1/n^s$ and with the same arguments as in [BK] Proposition 6.4, the above identity can be justified for all (s_1, \dots, s_l) with $s_1 > 1$. Related definition for q -analogues of multiple zeta values are given in [Br], [Ta], [Zu] and [OOZ]. It is convenient to define $Z_Q(\emptyset) = 1$ and then we denote the vector space spanned by all these elements by

$$Z(Q, S) := \langle Z_Q(s_1, \dots, s_l) \mid l \geq 0 \text{ and } s_1, \dots, s_l \in S \rangle_{\mathbb{Q}}. \quad (2.2)$$

Note by the above convention we have that \mathbb{Q} is contained in this space.

Lemma 2.1. If for each $r, s \in S$ there exists numbers $\lambda_j(r, s) \in \mathbb{Q}$ such that

$$Q_r(t) \cdot Q_s(t) = \sum_{\substack{j \in S \\ 1 \leq j \leq r+s}} \lambda_j(r, s) (1 - t)^{r+s-j} Q_j(t), \quad (2.3)$$

then the vector space $Z(Q, S)$ is a \mathbb{Q} -algebra,

Proof. We have to show that $Z_Q(s_1, \dots, s_l) \cdot Z_Q(r_1, \dots, r_m) \in Z(Q, S)$ and illustrate this in the $l = m = 1$ case because the higher length case will be clear after this. Suppose there is a representation of the form (2.3) then it is

$$\begin{aligned} Z_Q(r) \cdot Z_Q(s) &= \sum_{n_1 > 0} \frac{Q_r(q^{n_1})}{(1 - q^{n_1})^r} \cdot \sum_{n_2 > 0} \frac{Q_s(q^{n_2})}{(1 - q^{n_2})^s} \\ &= \sum_{n_1 > n_2 > 0} \cdots + \sum_{n_2 > n_1 > 0} \cdots + \sum_{n_1 = n_2 = n > 0} \frac{Q_r(q^n)Q_s(q^n)}{(1 - q^n)^{r+s}} \\ &= Z_Q(r, s) + Z_Q(s, r) + \sum_{j \in S'} \lambda_j Z_Q(j) \in Z(S, Q). \end{aligned}$$

□

We give three examples of q -analogues of multiple zeta values, which are currently considered by different authors where just the second and the third will be of interest in the rest of this note.

0) The polynomials $Q_s^T(t) = t^{s-1}$ are considered in [Ta] and sums of the form (2.1) with $s_1 > 1$ and $s_2, \dots, s_l \geq 1$ are studied there.

i) In [BK] the authors choose $Q_s^E(t) = \frac{1}{(s-1)!} t P_{s-1}(t)$, where the $P_s(t)$ are the eulerian polynomials defined by

$$\frac{t P_{s-1}(t)}{(1-t)^s} = \sum_{d=1}^{\infty} d^{s-1} t^d$$

for $s \geq 0$. With this define for all $s_1, \dots, s_l \in \mathbb{N}$

$$[s_1, \dots, s_l] := \sum_{n_1 > \dots > n_l > 0} \prod_{j=1}^l \frac{Q_{s_j}^E(q^{n_j})}{(1 - q^{n_j})^{s_j}}.$$

and set

$$\mathcal{MD} = Z(\{Q_s^E(t)\}_s, \mathbb{N}).$$

These *brackets* are generating functions for multiple divisor sums and they occur in the Fourier expansion of multiple Eisenstein series.

ii) Okounkov chooses the following polynomials in [Ok]

$$Q_s^O(t) = \begin{cases} t^{\frac{s}{2}} & s = 2, 4, 6, \dots \\ t^{\frac{s-1}{2}} (1+t) & s = 3, 5, 7, \dots \end{cases}$$

and defines for $s_1, \dots, s_l \in S = \mathbb{N}_{>1}$

$$Z(s) = \sum_{n_1 > \dots > n_l > 0} \prod_{j=0}^l \frac{Q_{s_j}^O(q^{n_j})}{(1 - q^{n_j})^{s_j}}.$$

We write for the space of the Okounkov q -multiple zetas

$$\mathfrak{qMZV} = Z(\{Q_s^O(t)\}_s, \mathbb{N}_{>1}).$$

Proposition 2.2. For the polynomials above we have

i) for $r, s \in \mathbb{N}$ and $Q_j^E(t) = \frac{1}{(s-1)!} t P_{s-1}(t)$

$$Q_r^E(t) \cdot Q_s^E(t) = \sum_{j=1}^r \lambda_{r,s}^j (1-t)^{r+s-j} Q_j^E(t) + \sum_{j=1}^s \lambda_{s,r}^j (1-t)^{r+s-j} Q_j^E(t) + Q_{r+s}^E(t),$$

where the coefficient $\lambda_{a,b}^j \in \mathbb{Q}$ for $1 \leq j \leq a$ is given by

$$\lambda_{a,b}^j = (-1)^{b-1} \binom{a+b-j-1}{a-j} \frac{B_{a+b-j}}{(a+b-j)!}.$$

ii) for $r, s \in \mathbb{N}_{>1}$ it is

$$Q_r^O(t) \cdot Q_s^O(t) = \begin{cases} Q_{r+s}^O(X) & , r, s \text{ even or } r+s \text{ odd} \\ 4Q_{r+s}^O(t) + (1-t)^2 Q_{r+s-2}^O(t) & , r, s \text{ odd.} \end{cases}$$

In particular, because of Lemma 2.1, the vector spaces \mathcal{MD} and \mathfrak{qMZV} are \mathbb{Q} -algebras.

Proof. In [BK] the claim i) is proven. The cases in ii) are checked easily. \square

Corollary 2.3. $\mathcal{MD}^\sharp = Z(\{Q_s^E\}_s, \mathbb{N}_{>1})$ is a sub algebra of \mathcal{MD} .

Proof. Using Proposition 2.2 it is easy to see that it suffices to show that

$$\lambda_{a,b}^1 + \lambda_{b,a}^1 = ((-1)^{a-1} + (-1)^{b-1}) \binom{a+b-2}{a-1} \frac{B_{a+b-1}}{(a+b-1)!}$$

vanishes for $a, b > 1$. This term clearly vanishes when a and b have different parity. In the other case $a+b-1$ is odd and greater than 1, as $a, b > 1$. It is well known that in this case $B_{a+b-1} = 0$, from which we deduce that $\lambda_{a,b}^1 + \lambda_{b,a}^1 = 0$. \square

Theorem 2.4. Let $Z(Q, \mathbb{N}_{>1})$ be any family of q -analogues of multiple zeta values as in (2.2), where each $Q_s(t) \in Q$ is a polynomial with degree at most $s - 1$, then

$$Z(Q, \mathbb{N}_{>1}) = \mathcal{MD}^\# .$$

and therefore all such families of q -analogues of multiple zeta values are \mathbb{Q} -subalgebras of \mathcal{MD} . In particular $\mathfrak{qMZV} = \mathcal{MD}^\#$.

Proof. To prove the first equality it is sufficient to show that for each $s > 1$ there are numbers $\lambda_j \in \mathbb{Q}$ with $2 \leq j \leq s$ such that

$$\frac{Q_s(t)}{(1-t)^s} = \sum_{j=2}^s \lambda_j \frac{Q_j^E(t)}{(1-t)^j} .$$

The space of polynomials with at most degree $s - 1$ and no constant term has dimension $s - 1$. For $2 \leq j \leq s$ the polynomials $(1-t)^{s-j} Q_j'(t)$ are all linear independent since $Q_j'(1) \neq 1$ and therefore such λ_j exist. The second statement follows directly from the definition of \mathfrak{qMZV} . \square

The following proposition allows one to write an arbitrary element in $Z(Q, \mathbb{N}_{>1})$ as an linear combination of $[s_1, \dots, s_l] \in \mathcal{MD}^\#$.

Proposition 2.5. Assume $k \geq 2$. For $1 \leq i, j \leq k - 1$ define the numbers $b_{i,j}^k \in \mathbb{Q}$ by

$$\sum_{j=1}^{k-1} \frac{b_{i,j}^k}{j!} t^j := \binom{t+k-1-i}{k-1} .$$

With this it is for $1 \leq i \leq k - 1$ and $Q_j^E(t) = \frac{1}{(j-1)!} t P_j(t)$

$$t^i = \sum_{j=2}^k b_{i,j-1}^k (1-t)^{k-j} Q_j^E(t) .$$

Proof. We want to show that

$$\frac{t^i}{(1-t)^k} = \sum_{j=1}^{k-1} \frac{b_{i,j}^k}{j!} \frac{t P_j(t)}{(1-t)^{j+1}}$$

By the definition of the Eulerian Polynomials it is

$$\begin{aligned} \sum_{j=1}^{k-1} \frac{b_{i,j}^k}{j!} \frac{t P_j(t)}{(1-t)^{j+1}} &= \sum_{j=1}^{k-1} \frac{b_{i,j}^k}{j!} \sum_{d>0} d^j t^d \\ &= \sum_{d>0} \left(\sum_{j=1}^{k-1} \frac{b_{i,j}^k}{j} d^j \right) t^d \\ &= \sum_{d>0} \binom{d-i+k-1}{k-1} t^d \end{aligned}$$

The claim now follows directly from the easy to prove formula

$$\frac{1}{(1-t)^k} = \sum_{n \geq 0} \binom{n+k-1}{k-1} t^n.$$

□

We give some examples how to write elements in \mathfrak{qMZV} as linear combinations of elements in \mathcal{MD} . From the proposition we deduce for the length one case for all $k > 0$

$$Z(2k) = \sum_{j=2}^{2k} b_{k,j-1}^{2k} [j] \quad \text{and} \quad Z(2k+1) = \sum_{j=2}^{2k+1} (b_{k,j-1}^{2k+1} + b_{k+1,j-1}^{2k+1}) [j].$$

Clearly this also suffices to give linear combinations in higher length.

Example 2.6. We give some examples

$$\begin{aligned} Z(2) &= [2], & Z(3) &= 2[3], \\ Z(4) &= [4] - \frac{1}{6}[2], & Z(5) &= 2[5] - \frac{1}{6}[3], \\ Z(6) &= [6] - \frac{1}{4}[4] + \frac{1}{30}[2], & Z(7) &= 2[7] - \frac{1}{3}[5] + \frac{1}{45}[3], \\ Z(2,2) &= [2,2], & Z(2,4) &= [2,4] - \frac{1}{6}[2,2]. \end{aligned}$$

The q -expansion of modular forms are well known to give rise to q -analogues of Riemann zeta values. Let us denote by $M_{\mathbb{Q}} = \mathbb{Q}[G_4, G_6]$ and $\widetilde{M}_{\mathbb{Q}} = \mathbb{Q}[G_2, G_4, G_6]$ the ring of modular and quasi-modular forms, where the Eisenstein series G_2 , G_4 and G_6 are given by

$$G_2 = -\frac{1}{24} + [2], \quad G_4 = \frac{1}{1440} + [4], \quad G_6 = -\frac{1}{60480} + [6].$$

We clearly have the following inclusions of \mathbb{Q} -algebras

$$M_{\mathbb{Q}} \subset \widetilde{M}_{\mathbb{Q}} \subset \mathfrak{qMZV} \subset \mathcal{MD}.$$

where the second inclusion follows from

$$\begin{aligned} G_2 &= -\frac{1}{24} + Z(2), \\ G_4 &= \frac{1}{1440} + Z(2) + \frac{1}{6}Z(4), \\ G_6 &= -\frac{1}{60480} + Z(6) + \frac{1}{4}Z(4) + \frac{1}{120}Z(2). \end{aligned}$$

In the theory of modular forms the operator $d := q \frac{d}{dq}$ plays an important role and it is a well known fact that $\widetilde{\mathcal{M}}_Q$ is closed under d . In [BK] the authors showed the following

Theorem 2.7. The operator d is a derivation on \mathcal{MD} that is compatible with the filtrations on \mathcal{MD} given by the weight and the length.

In [Ok] the following conjecture is stated by Okounkov

Conjecture 2.8. The operator d is a derivation on \mathfrak{qMZV} .

For the derivative of a length one generating series of multiple divisor sums we have several identities. These will be used to make the following result which gives some evidence for the conjecture above.

Proposition 2.9. It is $dZ(k) \in \mathfrak{qMZV}$ for all $k \geq 2$.

Proof. In [BK] Theorem 3.5 the authors prove the following representation of the derivative $d[k-2]$

$$\begin{aligned} \binom{k-2}{s_1-1} \frac{d[k-2]}{k-2} &= [s_1] \cdot [s_2] - [s_1, s_2] - [s_2, s_1] \\ &+ \binom{k-2}{s_1-1} [k-1] - \sum_{\substack{a+b=k \\ a>s_1}} \left(\binom{a-1}{s_1-1} + \binom{a-1}{s_2-1} - \delta_{a,s_2} \right) [a, b]. \end{aligned}$$

where $s_1, s_2 > 0$ can be chosen arbitrary such that $k = s_1 + s_2$. First divide both sides by $\binom{k-2}{s_1-1} (k-2)^{-1}$. Whenever $k \geq 4$ all elements on the right of the resulting equation belong to \mathcal{MD}^\sharp except for the term with $[k-1, 1]$. By direct calculation one obtains that for $s_1 = 1$ and $s_2 = k-1$ the coefficient of $[k-1, 1]$ is $-(k-2)$ and for $s_2 = 2$ and $s_1 = k-2$ it is $-2(k-2)$ and therefore $d[k-2]$ can be expressed as an element in \mathcal{MD}^\sharp . \square

Since d is a derivation it satisfies the Leibniz rule. Therefore the above proposition allows us to derive further identities, e.g.

$$dZ(k, \dots, k), d(Z(k_1, k_2) + Z(k_2, k_1)) \in \mathfrak{qMZV}.$$

Example 2.10. Some examples of representations of $dZ(s)$ in $qMZV$.

$$\begin{aligned}
dZ(2) &= 3Z(4) + Z(2) - Z(2, 2), \\
dZ(3) &= 5Z(5) + Z(3) - 4Z(3, 2) - 6Z(2, 3), \\
dZ(4) &= 10Z(6) + 2Z(4) + 4Z(4, 2) - 8Z(2, 4) - 6Z(3, 3), \\
dZ(2, 2) &= -6Z(6) - 12Z(2, 2, 2) - 15Z(4, 2) + 3Z(2, 4) + 9Z(3, 3), \\
dZ(3, 3) &= 4Z(8) - 12Z(2, 3, 3) - 10Z(3, 2, 3) - 8Z(3, 3, 2) \\
&\quad + Z(3, 5) - Z(5, 3) + 8Z(6, 2) + 3Z(3, 3), \\
dZ(2, 2, 2) &= -24Z(2, 2, 2, 2) + 9Z(2, 3, 3) + 9Z(3, 2, 3) + 6Z(3, 3, 2) \\
&\quad - 15Z(4, 2, 2) - 15Z(2, 4, 2) + 3Z(2, 2, 4) - 6Z(2, 6) + 6Z(5, 3) - 6Z(6, 2).
\end{aligned}$$

At the end we give some conjectured representations of $dZ(s)$ in $qMZV$ coming from numerical experiments and which were checked for the first 200 coefficients but which should be also provable by using the results in [BK].

$$\begin{aligned}
dZ(2, 3) &= 2Z(7) - 16Z(2, 2, 3) - 4Z(2, 3, 2) - 8Z(3, 2, 2) \\
&\quad - 15Z(4, 3) - 4Z(3, 4) + 4Z(5, 2) + 5Z(2, 5) + Z(3, 2) - Z(2, 3),
\end{aligned}$$

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E-mail:

henrik.bachmann@uni-hamburg.de

FACHBEREICH MATHEMATIK (AZ)

UNIVERSITÄT HAMBURG

BUNDESSTRASSE 55

D-20146 HAMBURG

Danksagung

Zunächst möchte ich mich bei meinem Doktorvater Prof. Dr. Ulf Kühn für seine engagierte und hilfreiche Betreuung bedanken. Seit meinem Bachelorstudiums hat er mich in allen Bereichen meines Studiums unterstützt und gefördert. Mehrfach haben seine Ideen meine Arbeiten in die richtigen Richtungen gelenkt und seine Erfahrungen im wissenschaftlichen Arbeiten hat er großzügig mit mir geteilt. Die durch ihn geschaffene Arbeitsatmosphäre habe ich als sehr angenehm empfunden, so dass ich gerne in seiner Arbeitsgruppe mitgewirkt habe. Don Zagier und Wadim Zudilin danke ich für das Interesse an meiner Dissertation und dafür, dass sie sich stets Zeit für mich genommen haben, wenn wir uns auf Konferenzen getroffen haben.

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Meiner Schwester Inger Maleen Bachmann danke ich für sorgfältiges Lesen und Korrigieren meiner Arbeit. Abschließend möchte ich meinen Eltern für ihre jahrelange Unterstützung während meines gesamten Studiums danken.

Zusammenfassung

Diese Arbeit beschäftigt sich mit Multiplen Eisensteinreihen, die einen Zusammenhang zwischen Multiplen Zeta-Werten und Modulformen liefern. Multiple Zeta-Werte sind Verallgemeinerungen der Riemansschen Zeta-Werte, die eine Vielzahl von \mathbb{Q} -linearen Relationen erfüllen. In ähnlicher Weise sind die von Gangl, Kaneko und Zagier eingeführten Multiplen Eisensteinreihen Verallgemeinerungen der klassischen Eisensteinreihen. Multiple Eisensteinreihen besitzen eine Fourierentwicklung bestehend aus Produkten von Multiplen Zeta-Werten und bestimmten q -Reihen, die als Brackets bezeichnet werden.

Aus Konvergenzgründen gibt es mehr Multiple Zeta-Werte als Multiple Eisensteinreihen. Das Ziel dieser Arbeit war es daher, die bisher bekannte Definition durch eine geeignete Regularisierung Multipler Eisensteinreihen zu erweitern. Dafür wird die Fourierentwicklung dieser Reihen genauer untersucht und insbesondere die Algebra Struktur der dort auftretenden Brackets betrachtet.

Es wird gezeigt, dass die Algebra-Struktur dieser Brackets ähnlich ist zu der von Multiplen Zeta-Werten und dass der Raum aller Brackets abgeschlossen ist unter dem Operator $q \frac{d}{dq}$. Ähnlich zu den Multiplen Zeta-Werten erfüllen diese q -Reihen auch viele \mathbb{Q} -lineare Relationen. Diese Relationen können auf eine rein kombinatorische Art beschrieben werden, indem die Brackets zu sogenannten Bi-Brackets verallgemeinert werden.

Es wird gezeigt, dass die Fourierentwicklung Multipler Eisensteinreihen eine direkte Verbindung zu dem Koproduct von formalen Iterierten Integralen besitzt. Mit Hilfe der Algebra Struktur der Bi-Brackets und diesem Zusammenhang werden zwei Arten von regularisierten Multiplen Eisensteinreihen angegeben.

Während der Untersuchung der Brackets stellt sich außerdem heraus, dass diese q -Reihen auch als q -Analoge von Multiplen zeta-Werten betrachtet werden können. Dies liefert, neben den Multiplen Eisensteinreihen, eine weitere direkte Verbindung von Modulformen zu Multiplen Zeta-Werten.

Abstract

This thesis studies a specific connection of multiple zeta values and modular forms given by multiple Eisenstein series. Multiple zeta values are real numbers being natural generalizations of the Riemann zeta values fulfilling a large class of \mathbb{Q} -linear relations. In a similar way multiple Eisenstein series are a generalizations of classical Eisenstein series studied by Gangl, Kaneko and Zagier. These functions have a Fourier expansions that consists of products of multiple zeta values and certain q -series, called brackets.

Due to convergence reasons there are more multiple zeta values than multiple Eisenstein series. The goal of this thesis was to give an extended definition of regularized multiple Eisenstein series by studying the Fourier expansion of multiple Eisenstein series and in particular the algebraic structure of the brackets.

It is shown that the space of brackets have a similar algebraic structure as the space of multiple zeta values and that it is closed under the differential operator $q \frac{d}{dq}$. Similar to multiple zeta values the brackets fulfill a lot of \mathbb{Q} -linear relations. These linear relations can be described in a combinatorial way by extending the space of brackets to a larger class of q -series called bi-brackets.

Using this algebraic structure together with a connection of the coproduct of formal iterated integrals to the Fourier expansion of multiple Eisenstein series, we define two types of regularized multiple Eisenstein series.

Besides their appearance in the Fourier expansion, the brackets can also be seen as a q -analogue of multiple zeta values. This gives another direct connection of modular forms to multiple zeta values, since the space of modular forms is contained in the space of brackets.

Erklärung zum Eigenanteil

Folgende Arbeiten sind Bestandteil meiner kumulativen Dissertation "Multiple Eisenstein series and q -analogues of multiple zeta values".

i) The algebra of generating functions for multiple divisor sums and applications to multiple zeta values ([BK])

Zusammenarbeit mit: U. Kühn

Die Idee für diese Arbeit entstand zusammen mit Herrn Kühn aufbauend auf meiner Masterarbeit. Die Arbeit wurde unter anderem dazu genutzt, damit Herr Kühn mich in das Erstellen einer wissenschaftlichen Arbeit einarbeitet und betreut.

Die meisten Beweise und computerunterstützte Berechnungen, insbesondere die Algebra Struktur des Raumes \mathcal{MD} (Theorem 1.3) und die Abgeschlossenheit unter dem Operator d (Theorem 1.7), wurden dabei von mir entdeckt und ausgeführt. Einige Beweise wären aber ohne die Ideen von Herrn Kühn, zum Beispiel der Beweis von Theorem 1.13, nicht möglich gewesen.

Der Großteil des Aufbaus und die Aussagen der Sätze entstanden in vielen gemeinsamen Diskussionen, die dann von mir aufgeschrieben wurden.

ii) A short note on a conjecture of Okounkov about a q -analogue of multiple zeta values ([BK2])

Zusammenarbeit mit: U. Kühn

Diese Arbeit entstand, nachdem Okounkov ein Paper zu q -analogues von Multiplen Zeta Werten ins Arxiv hochgeladen hat. In gemeinsamen Diskussionen haben Herr Kühn und ich gesehen, dass die dort auftretenden Objekte eine Verbindung haben zu unseren q -

Reihen die wir in der ersten Arbeit behandelt haben. Ähnlich zu der ersten gemeinsamen Arbeit haben wir den Aufbau zusammen besprochen und ich die Beweis ausgeführt und aufgeschrieben.

iii) The double shuffle relations for multiple Eisenstein series ([BT])

Zusammenarbeit mit: K. Tasaka (Nagoya University, Japan)

Die Motivation für diese Arbeit entstand nach mehrfachen Diskussionen zusammen mit K. Tasaka auf zahlreichen Konferenzen. Die Frage nach einer Definition von multiplen Eisenstein Reihen für den Fall, in dem die ursprüngliche Definition als geordnete Summe nicht existiert, beschäftigte uns beide schon länger.

Dadurch motiviert wurde K. Tasaka im Sommer 2014 nach Hamburg eingeladen. In dieser Zeit haben wir zusammen die Grundlage für diese Arbeit, nämlich den Zusammenhang vom Koproduct formaler iterierter Integrale zur Fourierentwicklung von multiplen Eisensteinreihen, entdeckt und ausgearbeitet. Hierbei war die Konstruktion aus meiner Masterarbeit für die Berechnung der Fourierentwicklung multipler Eisensteinreihen ausschlaggebend. Die grundlegende Beweisidee, welche Teile des Koproductes zu welchem Teil in der Fourierentwicklung korrespondiert, haben wir zusammen in dieser Zeit anhand von Beispielen erarbeitet. Zusammen kamen wir in Diskussionen auch auf die Idee, diese Verbindung zu nutzen um die shuffle regularisierten multiplen Eisensteinreihen zu definieren, welches das zweite Hauptresultat der Arbeit darstellt.

Nach dem Besuch in Hamburg hat K. Tasaka begonnen die Arbeit in Japan aufzuschreiben und die Beweise für den allgemeinen Fall auszuführen. Im regen Emailaustausch mit mir und auf einer Konferenz Ende 2014 in Madrid haben wir die Arbeit gemeinsam zu Ende gebracht.

Hamburg, 12.10.2015

Eidesstattliche Erklärung

Ich versichere hiermit an Eides statt, dass ich die vorliegende Arbeit selbstständig verfasst und keine anderen als die angegebenen Hilfsmittel und Quellen verwendet habe.

Hamburg, 12.10.2015

Lebenslauf

- 22.04.1985 geboren in Hamburg
- 2004 Abitur in Hamburg
- 2004-2006 Studium Informatik Ingenieurwesen, TU Hamburg-Harburg
- 2006-2012 Studium der Mathematik, Universität Hamburg
- 2009 Bachelor of Science in Mathematik, Universität Hamburg
- 2012 Master of Science in Mathematik, Universität Hamburg
- 2012 Beginn der Promotion in Mathematik, Universität Hamburg
- seit 2012 wissenschaftlicher Mitarbeiter an der Universität Hamburg