Multiple zeta values and modular forms

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Lecture notes and videos are available at: `https://www.henrikbachmann.com/mzv2020.html`

These notes are under construction and therefore may contain mistakes and change without notice. If you find any typos/errors or have any suggestion, please let me know!

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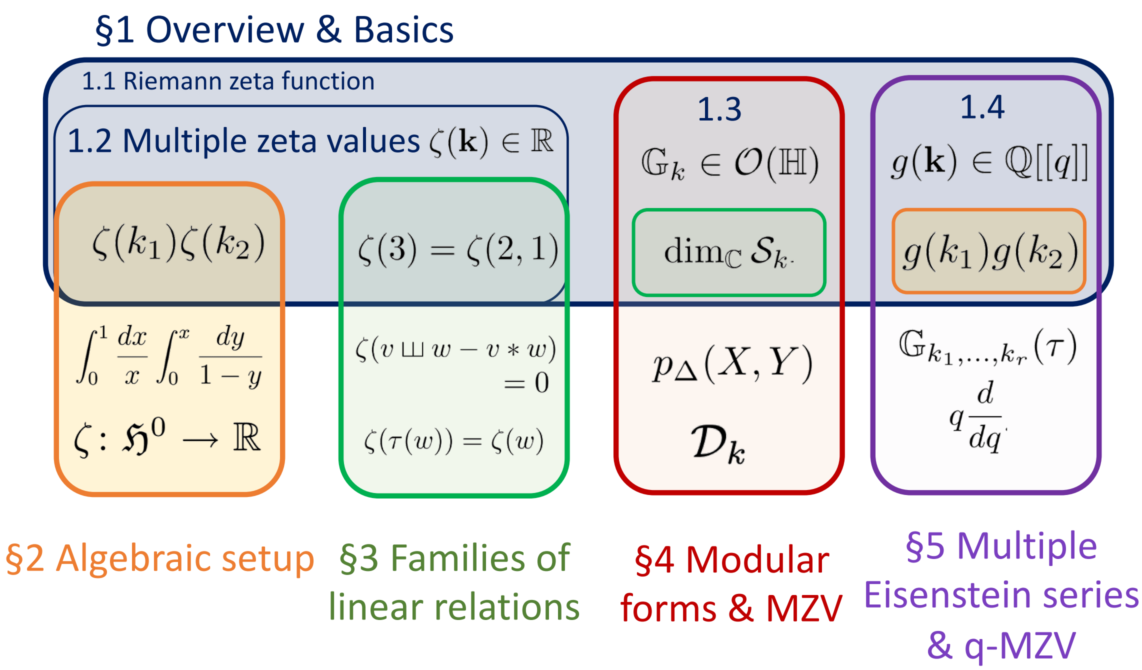
Introduction

In this course, we are interested in a **multiple** version of the Riemann **zeta** function and in the connection of their **values** at positive integer points to **modular forms**. We will mainly deal with three types of objects: Multiple zeta values (real numbers), modular forms (holomorphic functions in the complex upper half plane) and q-analogues of multiple zeta values (q-series with rational coefficients). The goal of this lecture is to describe some of the relationships between these objects, which were initiated by the beautiful work [GKZ]. There are various points of views from which one can study multiple zeta values and we will just be able to cover a small part of their exciting aspects. For more details on multiple zeta values we refer in particular to the books/lecture notes of Arakawa-Kaneko [AK], Burgos-Frésan [BF], Waldschmidt [W], Zhao [Zh1] and to the collection of Hoffman on research papers of multiple zeta values [H0].



A rough overview of the structure of these notes and the course.

The plan of this course is as follows: We start in Section 1 with an overview of almost all the objects we will deal with. First, we discuss the Riemann zeta function in (1.1), then introduce multiple zeta values (MZVs) in 1.2 and discuss some of their conjectures, algebraic structure and linear relations, which we then discuss in detail in Section 2 and 3. After this, we recall some basic facts on modular forms in 1.3 and state the Broadhurst-Kreimer conjecture, which gives the first indication of a connection of cusp forms and multiple zeta values. This connection will then be made precise in Section 4, where we present the main results of [GKZ]. In Section 1.4, we will introduce (some) q-analogues of multiple zeta values and show that they have a similar algebraic structure as multiple zeta values. This algebraic structure and its consequences will then be further described in Section 2 and 5.

§1 Overview & Basics

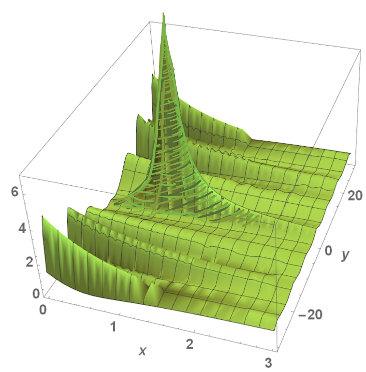
In this section, we will give an overview of the values of the Riemann zeta function, the definition of multiple zeta values, some of the main conjectures concerning their structure, and a glimpse of the connection of (q-analogues of) multiple zeta values and modular forms. The general picture of these concepts will be discussed in detail in the later Sections.

1.1 The values of the Riemann zeta function

The Riemann zeta function is defined for a complex variable $s \in \mathbb{C}$ with $\mathrm{Re}(s) > 1$ by

$$\zeta(s) = \sum_{m>0} \frac{1}{m^s}\,. \tag{1.1}$$

This function appears in various fields of mathematics and theoretical physics and it can be studied from various points of views. It plays a pivotal role in analytic number theory and has applications in physics, probability theory, and applied statistics.



The graph of $|\zeta(x+yi)|$ near the pole at $x+iy=1$.

For example, it is well-known that the Riemann zeta function can be analytically continued to the whole complex plane with a simple pole at $s = 1$. Even though $\zeta(s)$ was already considered by L. Euler (1707 – 1783), it was named after B. Riemann (1826 – 1866), who proved its meromorphic continuation and functional equation and established a relation between its zeros and the distribution of prime numbers.
In particular, he gave his famous conjecture on the location of the zeros of the Riemann zeta function, stating that besides the trivial zeros at $s = -2, -4, -6, \dots$ all other zeros have real part $\frac{1}{2}$.

The connection to prime numbers is given by the following product formula, which, to make things fair again, was named after Euler (Euler product formula)

$$\zeta(s) = \prod_{p \text{ prime}} \frac{1}{1-p^{-s}}\,. \qquad (\mathrm{Re}(s) > 1)$$

In this course, we will not study these analytic aspects but rather will be interested in the values of $\zeta(k)$, when $k \in \mathbb{Z}_{\geq 2}$ is a positive integer. The first result is the famous formula by Euler for $\zeta(2)$, which states that

$$\zeta(2) = \sum_{m>0} \frac{1}{m^2} = 1 + \frac{1}{4} + \frac{1}{9} + \frac{1}{16} + \cdots = \frac{\pi^2}{6}\,.$$

A sculpture of the pole of $\zeta(s)$ at $s = 1$ in front of Nagoya station in honor of the Riemann zeta function.

In general Euler proved that $\zeta(2m)$ is always a rational multiple of π^{2m} and he gave the following explicit formula in terms of Bernoulli numbers.

Proposition 1.1 (Euler, 1734)**.** *For all $m \in \mathbb{Z}_{\geq 1}$ we have*

$$\zeta(2m) = -\frac{B_{2m}}{2(2m)!}(2\pi i)^{2m} \in \mathbb{Q}\pi^{2m}\,,$$

where B_n denotes the n-th Bernoulli number defined by the Taylor expansion

$$\sum_{n=0}^{\infty} B_n \frac{x^n}{n!} = \frac{x}{e^x - 1}\,. \tag{1.2}$$

Proof. There are various ways to prove this fact and we will give the original approach due to Euler. First, consider the Weierstrass product of the sine function

$$\frac{\sin(\pi x)}{\pi x} = \prod_{n\geq 1}\left(1 - \frac{x^2}{n^2}\right). \tag{1.3}$$

For $x \in \mathbb{C}\backslash\mathbb{Z}$ we can take its logarithmic derivative to obtain the partial fraction expansion of the cotangent

$$\pi\cot(\pi x) = \frac{1}{x} + \sum_{n\geq 1}\left(\frac{1}{x+n} + \frac{1}{x-n}\right).$$

Expanding the right hand side in a geometric series gives

$$\frac{1}{x} + \sum_{n\geq 1}\left(\frac{1}{x+n} + \frac{1}{x-n}\right) = \frac{1}{x} - \sum_{m=1}^{\infty} 2\zeta(2m)x^{2m-1}\,.$$

On the other hand the left hand side can be evaluated as

$$\pi\cot(\pi x) = \pi i\frac{e^{\pi i x} + e^{-\pi i x}}{e^{\pi i x} - e^{-\pi i x}} = \pi i\left(1 + \frac{2}{e^{2\pi i x} - 1}\right) \overset{(1.2)}{=} \frac{1}{x} + \sum_{m=1}^{\infty}\frac{B_{2m}(2\pi i)^{2m}}{(2m)!}x^{2m-1}\,,$$

where in the last equality we used $B_1 = -\frac{1}{2}$. □

The first explicit values for $\zeta(2m)$ are given by the following

$$\zeta(2) = \frac{\pi^2}{6}\,,\quad \zeta(4) = \frac{\pi^4}{90}\,,\quad \zeta(6) = \frac{\pi^6}{945}\,,\quad \zeta(8) = \frac{\pi^8}{9450}\,,\quad \zeta(10) = \frac{\pi^{10}}{93555}\,,\quad \zeta(12) = \frac{691\pi^{12}}{638512875}\,.$$

Since π is transcendental (Lindemann, 1882), Proposition 1.1 gives the only family of polynomial relations among even zeta values. On the other hand, one does not expect polynomial relations among odd zetas. This is part of the following folklore conjecture.

Conjecture 1.2. *The numbers $1, \pi^2, \zeta(3), \zeta(5), \zeta(7), \dots$ are algebraically independent.*

So far there is not much known towards this conjecture. For the odd zeta values the following theorem gives an overview over the known facts.

Theorem 1.3. *i) $\zeta(3)$ is irrational.* (Apéry, 1978)

ii) For $m \geq 1$ we have

$$\dim_{\mathbb{Q}}\langle 1, \zeta(3), ..., \zeta(2m+1)\rangle \geq \frac{1}{3}\log(2m+1)\,.$$

In particular infinitely many of the values $\zeta(2m+1)$ are irrational. (Ball–Rivoal, 2001)

iii) At least one of the values $\zeta(5), \zeta(7), \zeta(9)$ and $\zeta(11)$ is irrational. (Zudilin, 2001)

1.2 Multiple zeta values

Due to Conjecture 1.2 we do not expect any linear relations among the values $\zeta(k_1)\zeta(k_2)$ if one of the k_i is odd. But it turns out that certain parts of these products satisfy numerous relations among each other. Splitting the product $\zeta(k_1)\zeta(k_2)$ into the following three parts leads us to the definition of the double zeta values $\zeta(k_1,k_2)$

$$\begin{aligned}\zeta(k_1)\zeta(k_2) = \sum_{m_1>0}\frac{1}{m_1^{k_1}}\sum_{m_2>0}\frac{1}{m_2^{k_2}} &= \left(\sum_{m_1>m_2>0}+\sum_{m_2>m_1>0}+\sum_{m_1=m_2>0}\right)\frac{1}{m_1^{k_1}m_2^{k_2}} \qquad (k_1,k_2\geq 2)\\ &=: \zeta(k_1,k_2)+\zeta(k_2,k_1)+\zeta(k_1+k_2)\,.\end{aligned} \tag{1.4}$$

For example we have the following expressions for the products of Riemann zeta values

$$\zeta(2)\zeta(5)=\zeta(2,5)+\zeta(5,2)+\zeta(7)\,,\qquad \zeta(3)\zeta(4)=\zeta(3,4)+\zeta(4,3)+\zeta(7)\,.$$

Even though we expect that there are no linear relations among $\zeta(2)\zeta(5)$ and $\zeta(3)\zeta(4)$, their "building blocks" given by $\zeta(7),\zeta(2,5),\zeta(3,4),\zeta(4,3)$ and $\zeta(5,2)$ satisfy various relations among each other. For example we will see (Exercise 1) that

$$\zeta(7)=4\zeta(3,4)+3\zeta(4,3)-2\zeta(5,2)\,. \tag{1.5}$$

Considering product of more than just two zeta values and using the same idea as in (1.4) leads us for integers $k_1,\dots,k_r$ to sums of the form

$$\sum_{m_1>\dots>m_r>0}\frac{1}{m_1^{k_1}\cdots m_r^{k_r}}\,. \tag{1.6}$$

Proposition 1.4. *For integers $k_1\geq 2$, $k_2,\dots,k_r\geq 1$ the sum (1.6) converges.*

Proof. It is enough to show the convergence for $k_1=2$ and $k_2=\dots=k_r=1$ for any r, since this gives an estimate for the other cases. Using the well-known inequality $\sum_{n=1}^{m}\frac{1}{n}\leq 1+\log(m)$ we obtain

$$\sum_{m_1>m_2>\dots>m_r>0}\frac{1}{m_1^2m_2\cdots m_r}=\sum_{m=1}^{\infty}\frac{1}{m^2}\sum_{m>m_2>\dots>m_r>0}\frac{1}{m_2\cdots m_r}\leq\sum_{m=1}^{\infty}\frac{1}{m^2}(1+\log(m))^{r-1}$$

and since $(1+\log(m))^{r-1}=o(\sqrt{m})$ as $m\to\infty$ for any r, the above sum converges. □

The multiple sum (1.6) will give the definition of the multiple zeta values which we will give after introducing the following notation.

Definition 1.5. *i) For $r\geq 0$ we call a tuple $\mathbf{k}=(k_1,\dots,k_r)\in\mathbb{Z}_{\geq1}^r$ of positive integers an* **index**. *For $r=0$ we write $\mathbf{k}=\emptyset$ and refer to it as the empty index.*

ii) An index $\mathbf{k}=(k_1,\dots,k_r)$ is called **admissible** *if $k_1\geq 2$ or $\mathbf{k}=\emptyset$.*

iii) For an index $\mathbf{k}=(k_1,\dots,k_r)$ we call $\mathrm{wt}(\mathbf{k})=k_1+\dots+k_r$ its **weight** *and $\mathrm{dep}(\mathbf{k})=r$ its* **depth**. *We set $\mathrm{wt}(\emptyset)=\mathrm{dep}(\emptyset)=0$.*

Definition 1.6. *For an admissible index $\mathbf{k}=(k_1,\dots,k_r)$ we define the* **multiple zeta value** *$\zeta(\mathbf{k})$ by*

$$\zeta(\mathbf{k})=\zeta(k_1,\dots,k_r)=\sum_{m_1>\dots>m_r>0}\frac{1}{m_1^{k_1}\cdots m_r^{k_r}}\in\mathbb{R}$$

and $\zeta(\emptyset)=1$. In the case $r=1$ (resp. $r=2$) we refer to these as single (resp. double) zeta values.

Remark 1.7. i) By Proposition 1.4 the $\zeta(\mathbf{k})$ gives for every admissible index $\mathbf{k}$ a real number. Even though the notion of weight and depth for these real numbers might not be well defined (and indeed we will see already in Proposition 1.8 below that this is not the case for the depth), we also say that $\zeta(\mathbf{k}) = \zeta(k_1, \dots, k_r)$ has weight $\mathrm{wt}(\mathbf{k}) = k_1 + \dots + k_r$ and depth $\mathrm{dep}(\mathbf{k}) = r$.

ii) For $r = 1$ the multiple zeta values are given by the values of the Riemann zeta function. One can also define multiple zeta functions $\zeta(s_1, \dots, s_r)$ for complex variables $s_1, \dots, s_r \in \mathbb{C}$ and consider their analytic properties similar to the classical case. See for example the thesis of Onozuka [On] for a nice detailed survey or [Zh1].

As we have seen before in an example, multiple zeta values satisfy various linear relations. The first one appears in weight 3 and is originally due to Euler. During the course we will see several ways to prove it and the interested reader can find 32 ways of doing so in [BB].

Proposition 1.8. *We have $\zeta(3) = \zeta(2, 1)$.*

Proof. The shortest proof known to the author is the following: Consider the following sum

$$S = \sum_{m,n>0} \frac{1}{mn(m+n)} = \sum_{m,n>0} \frac{1}{n^2}\left(\frac{1}{m} - \frac{1}{m+n}\right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{m=1}^{n} \frac{1}{m} = \zeta(3) + \zeta(2,1)\,.$$

This sum can also be evaluated as follows

$$S = \sum_{m,n>0} \left(\frac{1}{n} + \frac{1}{m}\right) \frac{1}{(m+n)^2} = \sum_{m,n>0} \frac{1}{n(m+n)^2} + \sum_{m,n>0} \frac{1}{m(m+n)^2} = 2\zeta(2,1)$$

and therefore the relation $\zeta(3) = \zeta(2, 1)$ follows. □

Another way to obtain relations among multiple zeta values is to evaluate the product $\zeta(k_1)\zeta(k_2)$ in two different ways. In (1.4) we saw that for $k_1, k_2 \geq 2$

$$\zeta(k_1)\zeta(k_2) = \zeta(k_1, k_2) + \zeta(k_2, k_1) + \zeta(k_1 + k_2)\,, \tag{1.7}$$

which is often called the **stuffle product** (also called **harmonic product**). But we also have the following expression for the product, which is called the **shuffle product**.

Proposition 1.9. *For $k_1, k_2 \geq 2$ we have*

$$\zeta(k_1)\zeta(k_2) = \sum_{j=2}^{k_1+k_2-1} \left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1}\right) \zeta(j, k_1 + k_2 - j)\,, \tag{1.8}$$

where we use the usual convention $\binom{n}{k} = 0$ for $n < k$.

Proof. This is Exercise 1 and can be done by using partial fraction decomposition. □

Comparing the right hand sides of (1.7) and (1.8) gives for $k_1, k_2 \geq 2$ a linear relation among multiple zeta values, which is an example for a so-called **(finite) double shuffle relation**. We will consider the stuffle/harmonic & shuffle product and the resulting double shuffle relations in detail for arbitrary depth in Section 2 and 3.

Example 1.10. *For $k_1 = 2$, $k_2 = 3$ equations (1.7) and (1.8) give*

$$\zeta(2)\zeta(3) = \zeta(2,3) + \zeta(3,2) + \zeta(5)\,,$$
$$\zeta(2)\zeta(3) = \zeta(2,3) + 3\zeta(3,2) + 6\zeta(4,1)\,,$$

from which we deduce the linear relation $\zeta(5) = 2\zeta(3,2) + 6\zeta(4,1)$.

We will denote the $\mathbb{Q}$-vector space spanned by all multiple zeta values by

$$\mathcal{Z} = \langle \zeta(\mathbf{k}) \mid \mathbf{k} \text{ admissible}\rangle_{\mathbb{Q}}\,.$$

For a fixed weight $k \geq 0$ we also define the space of weight k multiple zeta values by

$$\mathcal{Z}_k = \langle \zeta(\mathbf{k}) \mid \mathbf{k} \text{ admissible}, \mathrm{wt}(\mathbf{k}) = k\rangle_{\mathbb{Q}}\,.$$

Clearly we have $\mathcal{Z} = \sum_{k\geq 0} \mathcal{Z}_k$. With the same idea as in (1.4), where we showed that $\zeta(k_1)\zeta(k_2)$ is a linear combination of multiple zeta values of weight $k_1 + k_2$, we will see in Section 2 that this is true for arbitrary products of multiple zeta values and we will show the following (see Corollary 2.10).

Proposition 1.11. *The space $\mathcal{Z}$ is a $\mathbb{Q}$-subalgebra of $\mathbb{R}$ and we have $\mathcal{Z}_{k_1} \cdot \mathcal{Z}_{k_2} \subset \mathcal{Z}_{k_1+k_2}$ for $k_1, k_2 \geq 0$.*

All of the relations we saw so far: $\zeta(3) = \zeta(2,1)$, the relation (1.5), and the finite double shuffle relations are relations among multiple zeta values of the same weight. Indeed it is expected that there exist no $\mathbb{Q}$-linear relations among multiple zeta values of different weights, which is part of the following conjecture.

Conjecture 1.12. *The space $\mathcal{Z}$ is graded by weight, i.e.*

$$\mathcal{Z} = \bigoplus_{k\geq 0} \mathcal{Z}_k\,.$$

This conjecture is very strong as it implies (Exercise 2) the transcendence of every multiple zeta value of non-zero weight. One of the main interest in the theory of multiple zeta values is to understand all of their $\mathbb{Q}$-linear relations. There are several families of relations which conjecturally give all linear relations among multiple zeta values in a fixed weight. We will describe some of them in Section 3. In particular, we have a conjecture for the dimension of the spaces $\mathcal{Z}_k$, which was first observed by Zagier based on extensive numerical calculations. To state the conjecture we first introduce the integers d_k given by the following generating series

$$\sum_{k\geq 0} d_k X^k = \frac{1}{1 - X^2 - X^3}\,,$$

i.e. they are given by $d_0 = 1$, $d_1 = 0$, $d_2 = 1$ and the recursion $d_k = d_{k-2} + d_{k-3}$ for $k \geq 3$.

Conjecture 1.13 (Zagier, 1994)**.** *We have $\dim_{\mathbb{Q}} \mathcal{Z}_k = d_k$ for all $k \geq 0$.*

This conjecture shows that multiple zeta values satisfy a lot of linear relations. For example in weight $k = 14$ there are $2^{12} = 4096$ admissible indices (i.e. generators of $\mathcal{Z}_{14}$) and the conjectured dimension is $d_{14} = 21$. In the following we give a table for the number of admissible indices, the conjectured number of linearly independent relations and the numbers d_k.

weight k	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
# of adm. ind.	1	0	1	2	4	8	16	32	64	128	256	512	1024	2048	4096
# of relations $\stackrel{?}{=}$	0	0	0	1	3	6	14	29	60	123	249	503	1012	2032	4075
$\left(\dim_{\mathbb{Q}} \mathcal{Z}_k \stackrel{?}{=}\right) d_k$	1	0	1	1	1	2	2	3	4	5	7	9	12	16	21

Remark 1.14. One easy way to do numerical experiments for multiple zeta values is to use PARI/GP, which was actually the tool used by Zagier to come up with Conjecture 1.13 (It is available for free at `https://pari.math.u-bordeaux.fr/`). There the multiple zeta value $\zeta(k_1,\dots,k_r)$ is implemented as zetamult($[k_1,\dots,k_r]$) and the Riemann zeta function $\zeta(s)$ as zeta(s), which is of course the same as zetamult($[s]$). Together with the function lindep($[v_1,\dots,v_l]$) one can search for linear relations among the values $v_1,\dots,v_l$. For example to check if there is a relation between $\zeta(2,1)$ and $\zeta(3)$ one enters

```
input: lindep([zetamult([2,1]),zeta(3)])
output: [-1, 1]~
```

The output gives the coefficient of the relation $-1\cdot\zeta(2,1)+1\cdot\zeta(3)=0$. It is unknown if Euler also used PARI/GP to come up with $\zeta(2)=\frac{\pi^2}{6}$, but he could have done so by using

```
input: lindep([zeta(2),Pi^2])
output: [-6, 1]~
```

Of course these numerical calculations will not give a proof of any relations, since it is just a check up to a certain precision. But in any case an interested student should play around a little bit with these tools and maybe try to find nice relations and patterns, which he/she then could try to prove using the machinery we learn during this course.
If the coefficients in the output are extremely large, then this is an indication for the fact there are no $\mathbb{Q}$-linear relations among the values in the input. For example to check if there is a $\mathbb{Q}$-linear relation among $\zeta(3),\pi^3$ and 1 one enters

```
input: lindep([zeta(3),Pi^3,1])
output: [-5229795329281686, 216810578846293, -435977217249266]~
```

which indicates that there are (as expected) no relations among these values. The size of the numbers here depends on the current precision used, which can be changed by `\p 50` to, for example, set the precision to 50 significant digits.

The Conjecture 1.13 is out of reach at the moment and so far there is no weight k, for which we can actually prove that $\dim_{\mathbb{Q}}\mathcal{Z}_k>1$, since for example it is not even known (but expected) that $\zeta(5)$ and $\zeta(2,3)$ are linearly independent and that $\dim_{\mathbb{Q}}\mathcal{Z}_5=2$. Even though it seems to be impossible to give lower bounds for $\dim_{\mathbb{Q}}\mathcal{Z}_k$ so far, we know that the d_k give upper bounds:

Theorem 1.15 (Terasoma (2002), Deligne–Goncharov (2005)). *For all $k\geq 0$ we have $\dim_{\mathbb{Q}}\mathcal{Z}_k\leq d_k$.*

There also is a conjecture on an explicit basis for $\mathcal{Z}$ due to Hoffman.

Conjecture 1.16 (Hoffman [H1], 1997). *For $k\geq 0$ the multiple zeta values*

$$\{\zeta(k_1,\dots,k_r)\mid r\geq 0,\,k_1+\dots+k_r=k,\,k_1,\dots,k_r\in\{2,3\}\}$$

form a basis of $\mathcal{Z}_k$.

Notice that this conjecture would imply (Exercise 2) Zagiers dimension conjecture (Conjecture 1.13) since d_k counts exactly the number of indices of weight k with only 2's and 3's. Multiple zeta values with only 2's and 3's in their index will be called **Hoffman elements**. The linear independence of the Hoffman elements is unknown so far, but we know that these generate the whole space due to the following deep result of Brown.

Theorem 1.17 (Brown [Br], 2012). *For all $k\geq 0$ we have*

$$\mathcal{Z}_k=\langle\zeta(k_1,\dots,k_r)\mid r\geq 0,\,k_1+\dots+k_r=k,\,k_1,\dots,k_r\in\{2,3\}\rangle_{\mathbb{Q}}\,.$$

The only known proofs of Theorem 1.15 and 1.17 use deep concepts from algebraic geometry, particularly the theory of mixed Tate motives.

Remark 1.18. In his work [Br], Brown shows that all the above conjectures hold for so-called motivic multiple zeta values $\mathcal{Z}^{\mathfrak{m}}$, which are conjecturally isomorphic as a $\mathbb{Q}$-algebra to $\mathcal{Z}$. Using the surjective period map per : $\mathcal{Z}^{\mathfrak{m}} \twoheadrightarrow \mathcal{Z}$ Theorem 1.17 is then just a consequence of his more general results. For details on this, we refer to the excellent book [BF].

1.3 Modular forms and the Broadhurst-Kreimer conjecture

In this section we want to give a glimpse of the connection of modular forms and multiple zeta values and state the Broadhurst-Kreimer conjecture, which is a refinement of Zagiers dimensions conjecture (Conjecture 1.13). For this we will give a naive argument why cusp forms give rise to relations among double zeta values, which we will make precise later in Section 4. We will not give a complete introduction to modular forms and just state the main structure theorems and definitions. For a complete introduction to the theory of modular forms we refer the reader to [Za1] and [Za2].

1.3.1 Basics of modular forms

Let $\mathbb{H} = \{x + iy \in \mathbb{C} \mid x, y \in \mathbb{R}\,, y > 0\}$ denote the complex upper half plane. A holomorphic function $f \in \mathcal{O}(\mathbb{H})$ is called a **modular form of weight** $k \in \mathbb{Z}$ if it satisfies $f(\tau+1) = f(\tau)$, $f(-\frac{1}{\tau}) = \tau^k f(\tau)$ for all $\tau \in \mathbb{H}$ and if it has a Fourier expansion of the form

$$f(\tau) = \sum_{n=0}^{\infty} a_n q^n \qquad (a_n \in \mathbb{C})\,, \qquad q = q(\tau) = e^{2\pi i \tau}\,. \tag{1.9}$$

The map $q\colon \tau \mapsto \exp(2\pi i \tau)$ is the holomorphic map, which sends $\mathbb{H}$ to the punctured unit disc. The existence of (1.9) states that f, as a function in q, can be analytically continued to $q = 0$, and therefore give rise to a holomorphic function in the whole open unit disc $\{q \in \mathbb{C} \mid |q| < 1\}$. This is also equivalent to the fact that $f(\tau)$ is bounded as $\tau \to i\infty$.
By $\mathcal{M}_k$ we denote the **space of all modular forms of weight** k and we write $\mathcal{M} = \sum_{k \geq 0} \mathcal{M}_k$ for the space of all modular forms. It is easy to see that $\mathcal{M}$ equipped with the usual multiplication of holomorphic functions forms a $\mathbb{C}$-algebra. The coefficients $a_n \in \mathbb{C}$ in (1.9) are called the **Fourier coefficients** of f and a modular form for which $a_0 = 0$ (i.e. where the sum (1.9) starts at $n = 1$) is called a **cusp form**. We write

$$\mathcal{S}_k = \Big\{ f \in \mathcal{M}_k \mid f = \sum_{n=1}^{\infty} a_n q^n \Big\}$$

for the **space of all cusp forms of weight** k. The first non-trivial examples of modular forms are given by **Eisenstein series**, which are for even $k \geq 4$ defined by

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

For all even $k \geq 4$ we have $\mathbb{G}_k \in \mathcal{M}_k$. Notice that the above sum would vanish for odd k. In fact for all odd k we have $\mathcal{M}_k = 0$. The Fourier expansion of Eisenstein series, which we will calculate in Section 5.1 for a more general object, is given by

$$\mathbb{G}_k(\tau) = \zeta(k) + \frac{(-2\pi i)^k}{(k-1)!} \sum_{n=1}^{\infty} \sigma_{k-1}(n) q^n\,, \tag{1.10}$$

where $\sigma_{k-1}(n) = \sum_{d|n} d^{k-1}$ is the divisor sum. The expression (1.10) makes sense for any $k \geq 2$ and therefore we define $\mathbb{G}_k(\tau)$ for all $k \geq 2$ by (1.10). Though for $k = 2$ and odd k these are not modular forms of weight k anymore.
The Eisenstein series are the building blocks for all modular forms, and we summarize the main properties of modular forms in the following Theorem.

Theorem 1.19. *i) For even $k \geq 4$ we have $\mathcal{M}_k = \mathbb{C} \cdot \mathbb{G}_k \oplus \mathcal{S}_k$.*

ii) For odd, negative k or $k = 2$ we have $\mathcal{M}_k = 0$ and $\mathcal{M}_0 = \mathbb{C}$.

iii) For all $k_1, k_2 \geq 0$ we have $\mathcal{M}_{k_1} \cdot \mathcal{M}_{k_2} \subset \mathcal{M}_{k_1+k_2}$.

iv) The Eisenstein series $\mathbb{G}_4$ and $\mathbb{G}_6$ are algebraically independent (over $\mathbb{C}$).

v) We have

$$\mathcal{M} = \bigoplus_{k=0}^{\infty} \mathcal{M}_k = \mathbb{C}[\mathbb{G}_4, \mathbb{G}_6]\,,$$

i.e. $\mathcal{M}$ is a graded $\mathbb{C}$-algebra, which is isomorphic to the polynomial ring in two variables.

vi) The space $\mathcal{M}_k$ is generated by $\mathbb{G}_k$ and products of two Eisenstein series, i.e. for even $k \geq 4$

$$\mathcal{M}_k = \mathbb{C} \cdot \mathbb{G}_k + \langle \mathbb{G}_{k_1} \mathbb{G}_{k_2} \mid k_1, k_2 \geq 4 \text{ even}, k_1 + k_2 = k \rangle_{\mathbb{C}}\,.$$

Proof. The statements i), ii) & iii) follow almost immediately from the definition. Statement iv) and v) need some complex analysis and can be found in any standard book of modular forms (e.g. [B3],[Za2],[Za1]). The statement vi) follows from work of Rankin and can be found in [KZ]. □

The first non-trivial cusp form is the **discriminant function** Δ (a.k.a Ramanujan Delta function)

$$\Delta(\tau) = q \prod_{n=1}^{\infty} (1 - q^n)^{24} = q - 24q^2 + 252q^3 - 1472q^4 + \dots\,, \tag{1.11}$$

which is a cusp form $\Delta \in \mathcal{S}_{12}$ of weight 12. Since Δ has no zero in $\mathbb{H}$ and a zero of order one in $q = 0$, one can show that every cusp form of weight k can be written as a product of a modular form of weight $k - 12$ and Δ. Together with Theorem 1.19 this gives the following well-known theorem.

Theorem 1.20. *i) For $k \geq 0$ the map $\mathcal{M}_k \to \mathcal{S}_{k+12}$ given by $f \mapsto \Delta \cdot f$ is an isomorphism of $\mathbb{C}$-vector spaces.*

ii) The generating series for the dimension of cusp forms of weight k is given by

$$\mathsf{S}(X) = \sum_{k \geq 0} \dim_{\mathbb{C}} \mathcal{S}_k X^k = X^{12} \sum_{k \geq 0} \dim_{\mathbb{C}} \mathcal{M}_k X^k = \frac{X^{12}}{(1 - X^4)(1 - X^6)}\,.$$

1.3.2 The Broadhurst-Kreimer Conjecture

We now want to state a refinement of Conjecture 1.13 given by Broadhurst and Kreimer, which indicates a connection of cusp forms and the dimension of the depth graded spaces of multiple zeta values. The depth gives a filtration on the space $\mathcal{Z}$ and we write

$$\mathrm{Fil}^{\mathrm{D}}_r(\mathcal{Z}_k) = \langle \zeta(\mathbf{k}) \mid \mathbf{k} \text{ admissible}, \mathrm{wt}(\mathbf{k}) = k\,, \mathrm{dep}(\mathbf{k}) \leq r \rangle_{\mathbb{Q}}$$

for its depth r part and denote the associated graded part by $\mathrm{gr}^{\mathrm{D}}_r(\mathcal{Z}_k)$. In other words elements in $\mathrm{gr}^{\mathrm{D}}_r(\mathcal{Z}_k)$ are multiple zeta values of weight k and depth r modulo multiple zeta values of lower depth. For example the class of $\zeta(2,1)$ in $\mathrm{gr}^{\mathrm{D}}_2(\mathcal{Z}_3)$ is zero, since $\zeta(2,1) = \zeta(3)$.

Conjecture 1.21 (Broadhurst-Kreimer, 1997 [BroK]). *The generating series of the dimensions of the weight- and depth-graded parts of multiple zeta values is given by*

$$\sum_{k,r\geq 0} \dim_{\mathbb{Q}}\left(\operatorname{gr}^{\mathrm{D}}_r \mathcal{Z}_k\right) X^k Y^r = \frac{1+\mathsf{E}(X)Y}{1-\mathsf{O}(X)Y+\mathsf{S}(X)Y^2-\mathsf{S}(X)Y^4},$$

where

$$\mathsf{E}(X)=\frac{X^2}{1-X^2},\quad \mathsf{O}(X)=\frac{X^3}{1-X^2},\quad \mathsf{S}(X)=\sum_{k\geq 0}\dim_{\mathbb{C}}\mathcal{S}_k X^k=\frac{X^{12}}{(1-X^4)(1-X^6)}.$$

This conjecture reduces to Zagiers dimension conjecture (Exercise 2) by setting $Y=1$. Observe that

$$\frac{1+\mathsf{E}(X)Y}{1-\mathsf{O}(X)Y+\mathsf{S}(X)Y^2-\mathsf{S}(X)Y^4} = 1+\left(\mathsf{E}(X)+\mathsf{O}(X)\right)Y+\left(\left(\mathsf{E}(X)+\mathsf{O}(X)\right)\mathsf{O}(X)-\mathsf{S}(X)\right)Y^2+\cdots, \tag{1.12}$$

which indicates that cusp forms give rise to relation in depth 2. Before we make this more precise, we first want to give a naive reason why cusp forms give rise to linear relations among double zeta values. Let $f=\sum_{n=1}^{\infty}a_n q^n\in\mathcal{S}_k$ be a cusp form. By Theorem 1.19 vi) we know that f can be written for some $\alpha,\beta_{a,b}\in\mathbb{C}$ (we will just be interested in $\mathbb{Q}$) as

$$f=\alpha\mathbb{G}_k+\sum_{\substack{a,b\geq 4 \text{ even}\\ a+b=k}}\beta_{a,b}\mathbb{G}_a\mathbb{G}_b\,. \tag{1.13}$$

Considering the constant term in the Fourier expansion of both sides then yields the relation

$$0=\alpha\zeta(k)+\sum_{\substack{a,b\geq 4 \text{ even}\\ a+b=k}}\beta_{a,b}\zeta(a)\zeta(b)\,.$$

The products on the right hand side can now be evaluated by using either (1.7) or (1.8) to obtain a linear relation among double zeta values. This approach is not really interesting, since the representation of a cusp form (1.13) is not unique and also the choice of expanding the product is arbitrary. Therefore we can not really relate a cusp form to a single relation among double zeta values. But there is a surprising 1:1 correspondence between certain relations and cusp forms, which we will explain now.

For even weight k, the Broadhurst-Kreimer conjecture predicts by (1.12) that $\dim_{\mathbb{Q}}\left(\operatorname{gr}^{\mathrm{D}}_2\mathcal{Z}_k\right)$ is given by the coefficient of X^k in $\mathsf{O}(X)\,\mathsf{O}(X)-\mathsf{S}(X)$. The coefficent of $\mathsf{O}(X)\,\mathsf{O}(X)$ counts the number of indices (k_1,k_2) with $k_1,k_2\geq 3$ odd and $k_1+k_2=k$ for which we will write "(odd, odd)" in the following. If this would be the only contribution to $\dim_{\mathbb{Q}}\left(\operatorname{gr}^{\mathrm{D}}_2\mathcal{Z}_k\right)$ then a naive guess would be that the $\zeta(\text{odd},\text{odd})$ give a basis of $\operatorname{gr}^{\mathrm{D}}_2\mathcal{Z}_k$. Indeed, we will see in Section 4 that the $\zeta(\text{odd},\text{odd})$ span $\operatorname{gr}^{\mathrm{D}}_2\mathcal{Z}_k$. But the factor $\mathsf{S}(X)$ in the Broadhurst-Kreimer conjecture indicates that there are relations in weight k between these values whenever there exist cusp forms of weight k. The first relation between $\zeta(k_1,k_2)$, where both k_1 and k_2 are odd, appears in weight $k_1+k_2=12$ and is given by

$$-10394\zeta(3,9)+47650\zeta(5,7)+41431\zeta(7,5)-720\zeta(9,3)-10394\zeta(11,1)=0\,. \tag{1.14}$$

As shown in [GKZ] (See section 4) we have for all even $k\geq 4$ the relation

$$\sum_{\substack{k_1\geq 3, k_2\geq 1 \text{ odd}\\ k_1+k_2=k}}\zeta(k_1,k_2)=\frac{1}{4}\zeta(k)\,. \tag{1.15}$$

Combining the relations (1.14) and 1.15 gives

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

From this we get the following relation among $\zeta(\mathrm{odd},\mathrm{odd})$ in $\mathrm{gr}_2^{\mathrm{D}}\,\mathcal{Z}_{12}$

$$168\zeta(5,7)+150\zeta(7,5)+28\zeta(9,3)\equiv 0 \mod \zeta(12)\,.$$

In [GKZ] Gangl-Kaneko-Zagier give an explicit construction of such relations for a given cusp form $f\in\mathcal{S}_k$. For this they consider its period polynomial $p_f(X,Y)\in\mathbb{C}[X,Y]$ and show that one can obtain a relation among double zeta values explicitly from the coefficients of this polynomial (see Section 4.). For example the above relation can be obtain by taking for f a certain multiple of the cusp form Δ. A consequence of their results is the following.

Theorem 1.22. *(Gangl-Kaneko-Zagier, 2006) For even $k\geq 4$ the number of (independent) $\mathbb{Q}$-linear relations among $\zeta(2a+1,2b-1)$ with $a,b\geq 1$ and $k=2(a+b)$ is at least $\dim_{\mathbb{C}} S_k$.*

Conjecturally the number of these relations are exactly $\dim_{\mathbb{C}} S_k$. Due to a recent result of Tasaka [Tas], also a somehow converse statement is known: Given a relation among $\zeta(\mathrm{odd},\mathrm{odd})$ (which follows from a certain set of relations) of weight k, we can construct explicitly a cusp form of weight k. His result uses double Eisenstein series which we will discuss in Section 5.

1.4 q-analogues of multiple zeta values

A q-analogue of a theorem, identity or expression is a generalization involving a new parameter q that returns the original theorem, identity or expression in the limit as $q\to 1$[1]. The easiest example is the q-analogue of a natural number m given by the q-integer

$$[m]_q=\frac{1-q^m}{1-q}=1+q+\cdots+q^{m-1}\,,\qquad \lim_{q\to 1}[m]_q=m\,. \tag{1.16}$$

There are various different models of q-analogues of multiple zeta values in the literature. We will consider a few of them in this course and start with the most common model which was first independently studied by Bradley [Bra] and Zhao [Zh2]. For an admissible index $\mathbf{k}=(k_1,\dots,k_r)$ these are defined by

$$\zeta_q^{\mathrm{BZ}}(\mathbf{k})=\zeta_q^{\mathrm{BZ}}(k_1,\dots,k_r)=\sum_{m_1>\cdots>m_r>0}\frac{q^{(k_1-1)m_1}\cdots q^{(k_r-1)m_r}}{[m_1]_q^{k_1}\cdots[m_r]_q^{k_r}}\,. \tag{1.17}$$

By (1.16), together with a justification that one can interchange summation and taking the limit (see proof of Proposition 1.26), it is easy to see that we have

$$\lim_{q\to 1}\zeta_q^{\mathrm{BZ}}(\mathbf{k})=\zeta(\mathbf{k})\,.$$

In Section 3 we will see that these q-series satisfy a lot of relations which are satisfied by multiple zeta values. In particular, this is the unique model of q-analogues (in the sense we will define later) which satisfies the duality relation, e.g. $\zeta_q^{\mathrm{BZ}}(2,1)=\zeta_q^{\mathrm{BZ}}(3)$.

[1] Here and in the following we mean by $q\to 1$ the limit of q to 1 on the real axis with $|q|<1$.

In this course, we will mostly be interested in another model of q-analogues which is inspired by Eisenstein series and which was introduced by the author in his PhD-thesis [B2] and further studied in [BK1]. These objects are not q-analogues in the above sense, but are called often modified q-analogues. By a **modified q-analogue of weight k** we mean, that we first need to multiply by $(1-q)^k$ before taking the limit $q \to 1$. One motivation to consider modified q-analogues is the following.

Proposition 1.23. *Let $f(q) = \sum_{n=0}^{\infty} a_n q^n \in \mathcal{M}_k$ be a modular form of weight k. Then f is, up to the factor $(2\pi i)^k$, a modified q-analogue of weight k of its constant term a_0, i.e. we have*

$$\lim_{q\to 1}(1-q)^k f(q) = (2\pi i)^k a_0 \,.$$

Proof. This is a consequence of Proposition 1.26 below together with the fact that every modular form is a polynomial in $\mathbb{G}_4$ and $\mathbb{G}_6$. Another way to see this is by using the transformation property $f\left(-\frac{1}{\tau}\right) = \tau^k f(\tau)$. Taking the limit $q \to 1$ on the real axis corresponds to the limit $\tau \to 0$ on the positive imaginary axis, since $q = e^{2\pi i \tau}$. Together with $\lim_{\tau\to i\infty} f(\tau) = a_0$ we obtain

$$\lim_{q\to 1}(1-q)^k f(q) = \lim_{\tau\to 0}((2\pi i\tau)^k + O(\tau^{k+1}))f(\tau) = \lim_{\tau\to 0}(2\pi i)^k f\left(-\frac{1}{\tau}\right) = \lim_{\tau\to i\infty}(2\pi i)^k f(\tau) = (2\pi i)^k a_0 \,.$$

□

1.4.1 A modified q-analogue of multiple zeta values coming from Eisenstein series

For any $k \geq 2$ we defined in the previous section the Eisenstein series $\mathbb{G}_k(\tau)$ by its Fourier expansion

$$\mathbb{G}_k(\tau) = \zeta(k) + \frac{(-2\pi i)^k}{(k-1)!}\sum_{n=1}^{\infty}\sigma_{k-1}(n)q^n \,.$$

Clearly we can obtain $\zeta(k)$ from these series in the case $q \to 0$, but as indicated in Proposition 1.23 this will also be possible by considering $q \to 1$ after some modification. From now on we will always consider q as a formal variable or a fixed complex number with $|q| < 1$. Define for even $k \geq 2$ the q-series $G_k = (-2\pi i)^{-k}\mathbb{G}_k(\tau)$, then we have by Eulers formula $\zeta(2m) = -\frac{B_{2m}}{2(2m)!}(2\pi i)^{2m}$ (Proposition 1.1)

$$G_k = -\frac{B_k}{2k!} + \frac{1}{(k-1)!}\sum_{n=1}^{\infty}\sigma_{k-1}(n)q^n \in \mathbb{Q}[[q]] \,. \tag{1.18}$$

The right-hand side of (1.18) makes sense for any $k \geq 1$ and we will use it to define G_k for all $k \geq 2$. We will denote the constant term of G_k by $\beta(k) = -\frac{B_k}{2k!} \in \mathbb{Q}$ and denote the rest by

$$\mathrm{g}(k) = \frac{1}{(k-1)!}\sum_{n=1}^{\infty}\sigma_{k-1}(n)q^n \,,$$

i.e. $G_k = \beta(k) + \mathrm{g}(k)$. The $\mathrm{g}(k)$ can be rewritten in the following way

$$\mathrm{g}(k) = \frac{1}{(k-1)!}\sum_{n=1}^{\infty}\sigma_{k-1}(n)q^n = \sum_{m,d>0}\frac{d^{k-1}}{(k-1)!}q^{md} = \sum_{m>0}\frac{P_k(q^m)}{(1-q^m)^k} \,, \tag{1.19}$$

where for $k \geq 1$ the $P_k(X) \in \mathbb{Q}[X]$ are the **Eulerian polynomials**[2], defined by

$$\frac{P_k(X)}{(1-X)^k} = \sum_{d>0} \frac{d^{k-1}}{(k-1)!} X^d .$$

For $k = 1, \dots, 6$ these are given by

$$P_1(X) = P_2(X) = X, \quad P_3(X) = \frac{1}{2}X(X+1), \quad P_4(X) = \frac{1}{6}X(X^2+4X+1),$$
$$P_5(X) = \frac{1}{24}X(X+1)\left(X^2+10X+1\right), \quad P_6(X) = \frac{1}{120}X\left(X^4+26X^3+66X^2+26X+1\right).$$

Lemma 1.24. *For all $k \geq 1$ we have $P_k(0) = 0$ and $P_k(1) = 1$.*

Proof. This is Exercise 4 i). □

As a multiple version of the q-series $\mathrm{g}(k)$ in (1.19) we define the following.

Definition 1.25. *For any index $\mathbf{k} = (k_1, \dots, k_r) \in \mathbb{Z}^r_{\geq 1}$ we define*[3]

$$\mathrm{g}(\mathbf{k}) = \mathrm{g}(k_1, \dots, k_r) = \sum_{m_1 > \dots > m_r > 0} \frac{P_{k_1}(q^{m_1})}{(1-q^{m_1})^{k_1}} \cdots \frac{P_{k_r}(q^{m_r})}{(1-q^{m_r})^{k_r}} \in \mathbb{Q}[[q]] .$$

Notice that this is a well-defined q-series for any index (even when $k_1 = 1$) since $P_k(X) \in X\mathbb{Q}[X]$ (Lemma 1.24). These series can be seen as modified q-analogues of multiple zeta values, where by modified we mean that we need to multiply by a power of $(1-q)$ before taking the limit $q \to 1$.

Proposition 1.26. *For any admissible index $\mathbf{k}$ we have*

$$\lim_{q \to 1} (1-q)^{\mathrm{wt}(\mathbf{k})} \, \mathrm{g}(\mathbf{k}) = \zeta(\mathbf{k}) .$$

Proof. First we need to justify the interchange of summation and taking the limit, which follows from the fact that for $|q| < 1$ the sum inside the limit converges uniformly. We will skip the details and refer to [BK1, Lemma 6.6] for a precise proof. Then this is an easy consequence of Lemma 1.24 since for $k \geq 1$ we have

$$\lim_{q \to 1} (1-q)^k \frac{P_k(q^m)}{(1-q^m)^k} = \lim_{q \to 1} \frac{P_k(q^m)}{[m]_q^k} = \frac{P_k(1)}{m^k} = \frac{1}{m^k} .$$

□

We will denote the space spanned by all $\mathrm{g}(\mathbf{k})$ for any (not necessarily admissible!) index $\mathbf{k}$ by

$$\mathcal{G} = \left\langle \, \mathrm{g}(\mathbf{k}) \mid \mathbf{k} \text{ index} \right\rangle_{\mathbb{Q}} \subset \mathbb{Q}[[q]] ,$$

where we also use the convention $\mathrm{g}(\emptyset) = 1$. In Section 2 we will see (as a consequence of Lemma 2.18) that this space is also closed under multiplication and we will proof the following.

Proposition 1.27. *The space $\mathcal{G}$ is a $\mathbb{Q}$-subalgebra of $\mathbb{Q}[[q]]$.*

[2] In the literature usually $(k-1)!X^{-1}P_k(X)$ is called Eulerian polynomial.

[3] These q-series are called brackets in [BK1] and are denoted by $[k_1, \dots, k_r]$ there.

Similar as we did for multiple zeta values, we will show the lowest depth case of this proposition now. For $k_1, k_2 \geq 1$ we have, similar as in (1.4)

$$\begin{aligned}
\mathrm{g}(k_1)\,\mathrm{g}(k_2) &= \sum_{m_1>0} \frac{P_{k_1}(q^{m_1})}{(1-q^{m_1})^{k_1}} \sum_{m_2>0} \frac{P_{k_2}(q^{m_2})}{(1-q^{m_2})^{k_2}} \\
&= \left(\sum_{m_1>m_2>0} + \sum_{m_2>m_1>0} + \sum_{m_1=m_2>0} \right) \frac{P_{k_1}(q^{m_1})}{(1-q^{m_1})^{k_1}} \frac{P_{k_2}(q^{m_2})}{(1-q^{m_2})^{k_2}} \\
&= \mathrm{g}(k_1,k_2) + \mathrm{g}(k_2,k_1) + \sum_{m>0} \frac{P_{k_1}(q^{m})}{(1-q^{m})^{k_1}} \frac{P_{k_2}(q^{m})}{(1-q^{m})^{k_2}} \,.
\end{aligned} \tag{1.20}$$

That this is again an element in $\mathcal{G}$ follows now from the following lemma, which can be proven by using generating series together with the definition of the Bernoulli numbers (1.2).

Lemma 1.28. *For $k \geq 1$ we set $R_k(X) = \frac{P_k(X)}{(1-X)^k} = \sum_{d>0} \frac{d^{k-1}}{(k-1)!} X^d$. Then for all $k_1, k_2 \geq 1$ we have*

$$R_{k_1}(X) \cdot R_{k_2}(X) = R_{k_1+k_2}(X) + \sum_{j=1}^{k_1+k_2-1} \left(\lambda^j_{k_1,k_2} + \lambda^j_{k_2,k_1} \right) R_j(X) \tag{1.21}$$

where the rational numbers $\lambda^j_{k_1,k_2}$ are given by

$$\lambda^j_{k_1,k_2} = (-1)^{k_2-1} \binom{k_1+k_2-1-j}{k_1-j} \frac{B_{k_1+k_2-j}}{(k_1+k_2-j)!} \,,$$

and where we use the convention $\binom{n}{k} = 0$ for $k < 0$.

Proof. This is Exercise 4 ii). □

Lemma 1.28 together with (1.20) gives the following analogue for the q-series g of the stuffle product formula $\zeta(k_1)\zeta(k_2) = \zeta(k_1,k_2) + \zeta(k_2,k_1) + \zeta(k_1+k_2)$ of multiple zeta values.

Proposition 1.29. *For $k_1, k_2 \geq 1$ and we have*

$$\mathrm{g}(k_1)\,\mathrm{g}(k_2) = \mathrm{g}(k_1,k_2) + \mathrm{g}(k_2,k_1) + \mathrm{g}(k_1+k_2) + \sum_{j=1}^{k_1+k_2-1} \left(\lambda^j_{k_1,k_2} + \lambda^j_{k_2,k_1} \right) \mathrm{g}(j) \,.$$

Proof. This follows immediately by plugging (1.21) into (1.20). □

We see that the extra terms in the right-hand side are of lower weight and therefore these will vanish when multiplying both sides with $(1-q)^{k_1+k_2}$ and taking the limit $q \to 1$. In particular we see that this, together with Proposition 1.26, gives back the stuffle product formula for multiple zeta values. In contrast to $\mathcal{Z}$ (which is conjecturally graded by weight) the space $\mathcal{G}$ is therefore not graded by weight. We treat both of these products (for ζ and g) simultaneously in Section 3 as examples for a quasi-shuffle product. The series g also satisfy an analogue of the shuffle product formula

$$\zeta(k_1)\zeta(k_2) = \sum_{j=2}^{k_1+k_2-1} \left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1} \right) \zeta(j, k_1+k_2-j) \,,$$

which we saw in Proposition 1.30. This formula involves not just the series g but also its derivative with respect to the differential operator $q\frac{d}{dq}$.

Proposition 1.30. *For $k_1, k_2 \geq 1$ and $k = k_1 + k_2$ we have*

$$\begin{aligned} \mathrm{g}(k_1)\,\mathrm{g}(k_2) = &\sum_{j=1}^{k-1} \left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1} \right) \mathrm{g}(j, k-j) \\ &+ \binom{k-2}{k_1-1} \left(q\frac{d}{dq} \frac{\mathrm{g}(k-2)}{k-2} - \mathrm{g}(k-1) \right) + \delta_{k_1,1}\delta_{k_2,1}\,\mathrm{g}(2)\,, \end{aligned} \tag{1.22}$$

where $\delta_{i,j} = \begin{cases} 1\,, & i = j \\ 0\,, & i \neq j \end{cases}$ *denotes the Kronecker delta.*

We will give a proof of this formula by using generating series below. In general depth we will need, besides the derivative with respect to $q\frac{d}{dq}$, even more extra terms to get an analogue of the shuffle product. This will be discussed in Section 5.

Example 1.31. *i) Similar to the Example 1.10, where we showed*

$$\zeta(2)\zeta(3) = \zeta(2,3) + \zeta(3,2) + \zeta(5) = \zeta(2,3) + 3\zeta(3,2) + 6\zeta(4,1)\,, \tag{1.23}$$

we can use Propositions 1.29 and 1.30 to get the following formulas for the q-series g

$$\begin{aligned} \mathrm{g}(2)\,\mathrm{g}(3) &= \mathrm{g}(2,3) + \mathrm{g}(3,2) + \mathrm{g}(5) - \frac{1}{12}\,\mathrm{g}(3)\,, \\ \mathrm{g}(2)\,\mathrm{g}(3) &= \mathrm{g}(2,3) + 3\,\mathrm{g}(3,2) + 6\,\mathrm{g}(4,1) - 3\,\mathrm{g}(4) + q\frac{d}{dq}\,\mathrm{g}(3)\,. \end{aligned} \tag{1.24}$$

From this we deduce the linear relation $\mathrm{g}(5) = 2\,\mathrm{g}(3,2) + 6\,\mathrm{g}(4,1) + \frac{1}{12}\,\mathrm{g}(3) - 3\,\mathrm{g}(4) + q\frac{d}{dq}\,\mathrm{g}(3)$. *Multiplying equation (1.24) with $(1-q)^5$ and taking the limit $q \to 1$ gives the equation (1.23). This will be explained in detail in Section 5.*

ii) Since Propositions 1.29 and 1.30 are also valid for non admissible indices we get

$$\begin{aligned} \mathrm{g}(1)\,\mathrm{g}(2) &= \mathrm{g}(1,2) + \mathrm{g}(2,1) + \mathrm{g}(3) - \frac{1}{2}\,\mathrm{g}(2)\,, \\ \mathrm{g}(1)\,\mathrm{g}(2) &= \mathrm{g}(1,2) + 2\,\mathrm{g}(2,1) + q\frac{d}{dq}\,\mathrm{g}(1) - \mathrm{g}(2) \end{aligned}$$

by using $k_1 = 1, k_2 = 2$. This gives the following analogue of the relation $\zeta(3) = \zeta(2,1)$

$$\mathrm{g}(3) = \mathrm{g}(2,1) + q\frac{d}{dq}\,\mathrm{g}(1) - \frac{1}{2}\,\mathrm{g}(2)\,.$$

Since the $\mathrm{g}(k)$ are essentially, up to a constant, the Eisenstein series of weight k, above formulas can be used to give purely combinatorial proofs of identities among modular forms. One simple example is the identity $\mathbb{G}_4^2 = \frac{7}{6}\mathbb{G}_8$, which is a consequence of Proposition 1.29 and 1.30 (Exercise 4). In Section 4 we will elaborate on this combinatorial approach to modular forms.

1.4.2 Generating series

We now want to illustrate how the proofs of Proposition 1.29 and 1.30 can be done by using generating series. This will be done in more generality in Section 5, but we want to satisfy the curious reader.

The key point is, that there are two different ways to write the generating series of $\mathrm{g}(\mathbf{k})$. Multiplying one of them leads to the stuffle product and the other one to the shuffle product. For $r \geq 1$ we will denote the generating series of $\mathrm{g}(k_1,\dots,k_r)$ by

$$\mathfrak{g}(X_1,\dots,X_r) = \sum_{k_1,\dots,k_r\geq 1} \mathrm{g}(k_1,\dots,k_r) X_1^{k_1-1}\cdots X_r^{k_r-1}\,.$$

Lemma 1.32. *We have*

$$\mathfrak{g}(X_1,\dots,X_r) = \sum_{m_1>\dots>m_r>0} \frac{e^{X_1}q^{m_1}}{1-e^{X_1}q^{m_1}}\cdots\frac{e^{X_r}q^{m_r}}{1-e^{X_r}q^{m_r}} \tag{1.25}$$

$$= \sum_{m_1>\dots>m_r>0} \frac{e^{m_1X_r}q^{m_1}}{1-q^{m_1}}\frac{e^{m_2(X_{r-1}-X_r)}q^{m_2}}{1-q^{m_2}}\cdots\frac{e^{m_r(X_1-X_2)}q^{m_r}}{1-q^{m_r}}\,. \tag{1.26}$$

Proof. This is Exercise 5 i). The proof of (1.25) follows directly from the definition. For (1.26) a suitable change of summation variables is needed. □

Propositions 1.29 and 1.30 are a consequence of the following proposition by considering the coefficients of $X^{k_1-1}Y^{k_2-1}$. (Exercise 5 iii))

Proposition 1.33. *We have*

$$\mathfrak{g}(X)\mathfrak{g}(Y) = \mathfrak{g}(X,Y)+\mathfrak{g}(Y,X)+\frac{1}{e^{X-Y}-1}\mathfrak{g}(X)+\frac{1}{e^{Y-X}-1}\mathfrak{g}(Y) \tag{1.27}$$

$$= \mathfrak{g}(X+Y,X)+\mathfrak{g}(X+Y,Y)-\mathfrak{g}(X+Y)+q\frac{d}{dq}\sum_{k\geq 1}\mathrm{g}(k)\frac{(X+Y)^k}{k}+\mathrm{g}(2)\,. \tag{1.28}$$

Proof. Using (1.25) and (1.26) in the smallest depth case together with the usual splitting of the summation of $m_1, m_2 > 0$ into the cases $m_1 > m_2 > 0$, $m_2 > m_1 > 0$ and $m_1 = m_2 = m > 0$ gives

$$\mathfrak{g}(X)\mathfrak{g}(Y) \overset{(1.25)}{=} \mathfrak{g}(X,Y)+\mathfrak{g}(Y,X)+\sum_{m>0}\frac{e^Xq^m}{1-e^Xq^m}\frac{e^Yq^m}{1-e^Yq^m}\,,$$

$$\mathfrak{g}(X)\mathfrak{g}(Y) \overset{(1.26)}{=} \mathfrak{g}(X+Y,X)+\mathfrak{g}(X+Y,Y)+\sum_{m>0}e^{m(X+Y)}\left(\frac{q^m}{1-q^m}\right)^2\,.$$

It remains to evaluate the third term in both equations. For the first equation one can check by direct calculation that

$$\frac{e^Xq^m}{1-e^Xq^m}\frac{e^Yq^m}{1-e^Yq^m} = \frac{1}{e^{X-Y}-1}\cdot\frac{e^Xq^m}{1-e^Xq^m}+\frac{1}{e^{Y-X}-1}\cdot\frac{e^Yq^m}{1-e^Yq^m}\,,$$

which then gives

$$\mathfrak{g}(X)\mathfrak{g}(Y) = \mathfrak{g}(X,Y)+\mathfrak{g}(Y,X)+\frac{1}{e^{X-Y}-1}\mathfrak{g}(X)+\frac{1}{e^{Y-X}-1}\mathfrak{g}(Y)\,.$$

For the second equation one uses first $\left(\frac{q^m}{1-q^m}\right)^2 = \frac{q^m}{(1-q^m)^2}-\frac{q^m}{1-q^m}$, which gives

$$\sum_{m>0}e^{m(X+Y)}\left(\frac{q^m}{1-q^m}\right)^2 = \sum_{m>0}e^{m(X+Y)}\frac{q^m}{(1-q^m)^2}-\mathfrak{g}(X+Y)\,.$$

The first sum on the right can then be evaluated as (Exercise 5 ii))

$$\sum_{m>0} e^{m(X+Y)} \frac{q^m}{(1-q^m)^2} = \mathrm{g}(2) + q\frac{d}{dq} \sum_{k\geq 1} \mathrm{g}(k) \frac{(X+Y)^k}{k}\,, \tag{1.29}$$

from which the claimed formula follows. □

1.4.3 General modified q-analogues of multiple zeta values

As mentioned before, there are several models of q-analogues of multiple zeta values, and in [Zh3] you can find a nice overview of some of them. Most of these have similar definitions as the $\mathrm{g}(\mathbf{k})$ with the difference that the Eulerian polynomials get replaced by other polynomials. Also the modified version (by which we mean that we factor out the factor $(1-q)^{\mathrm{wt}(\mathbf{k})}$) of the Bradley-Zhao model $\zeta_q^{\mathrm{BZ}}(\mathbf{k})$ is of this form, since instead of $P_k(X)$ the polynomials X^{k-1} are used. In the following, we define a general type of q-analogue of multiple zeta values, which were introduced in [BK2].

Definition 1.34. *For $k_1,\dots,k_r \geq 1$ and polynomials $Q_1(X) \in X\mathbb{Q}[X]$ and $Q_2(X)\dots,Q_r(X) \in \mathbb{Q}[X]$ we define*

$$\zeta_q(k_1,\dots,k_r;Q_1,\dots,Q_r) = \sum_{m_1>\dots>m_r>0} \frac{Q_1(q^{m_1})\dots Q_r(q^{m_r})}{(1-q^{m_1})^{k_1}\cdots(1-q^{m_r})^{k_r}}\,. \tag{1.30}$$

Similar as in Proposition 1.26 these series can be seen as (modified) q-analogues of $\zeta(k_1,\dots,k_r)$, since we have for $k_1 \geq 2$

$$\lim_{q\to 1}(1-q)^{k_1+\dots+k_r}\zeta_q(k_1,\dots,k_r;Q_1,\dots,Q_r) = Q_1(1)\dots Q_r(1)\cdot\zeta(k_1,\dots,k_r)\,.$$

We only consider the case where $\deg(Q_j) \leq k_j$ and consider the following $\mathbb{Q}$-vector space:

$$\mathcal{Z}_q := \Big\langle \zeta_q(k_1,\dots,k_r;Q_1,\dots,Q_r) \;\Big|\; r\geq 0,\, k_1,\dots,k_r \geq 1,\, \deg(Q_j)\leq k_j \Big\rangle_{\mathbb{Q}}\,, \tag{1.31}$$

where again $\zeta_q(\emptyset;\emptyset) = 1$. It is again not hard to see that $\mathcal{Z}_q$ is a $\mathbb{Q}$-algebra, since it is again an example for a quasi-shuffle algebra (see Section 2.3.2), and we have for example

$$\zeta_q(k_1;Q_1)\zeta_q(k_2;Q_2) = \zeta_q(k_1,k_2;Q_1,Q_2) + \zeta_q(k_2,k_1;Q_2,Q_1) + \zeta_q(k_1+k_2;Q_1\cdot Q_2)\,.$$

Since $\mathrm{g}(k_1,\dots,k_r) = \zeta_k(k_1,\dots,k_r;P_{k_1},\dots,P_{k_r})$ and $\deg(P_k) \leq k$ we have $\mathcal{G} \subset \mathcal{Z}_q$. As we will see in the next section, we can describe the analogue of the stuffle product for elements in $\mathcal{G}$ and $\mathcal{Z}_q$ as examples of quasi-shuffle products. The reason to introduce the a priory bigger space $\mathcal{Z}_q$ is that we can describe the higher depth analogue of the shuffle product in this space. This we will do in Section 5. Even though we will not be able to describe the shuffle product analogue in the space $\mathcal{G}$ explicitly, we have the following surprising conjecture, which was discovered by the author during his PhD thesis.

Conjecture 1.35. *([B2], [BK2]) We have $\mathcal{G} = \mathcal{Z}_q$.*

If time permits we will discuss application and motiviations of this conjecture in Section 5.

§2 Algebraic setup

In this section we want to explain the algebraic structure of the spaces $\mathcal{Z}$ (multiple zeta values), $\mathcal{G}$ (the space of the q-analogues $g(\mathbf{k})$) and $\mathcal{Z}_q$ (q-analogues of multiple zeta values). In particular, we will see why these spaces are all $\mathbb{Q}$-algebras. For this we will introduce the algebraic setup of Hoffman, which was first introduced in [H1] and then later generalized to quasi-shuffle algebras in [HI].

2.1 Multiple polylogarithms, iterated integrals and duality

In the following we want to introduce the iterated integrals expression for multiple zeta values. This will be used in the next subsection to give another explanation of the shuffle product formula in (1.8). We start by calculating one simple example by hand, before giving a general formula afterwards. Consider the following iterated integral

$$\begin{aligned}\int_0^1 \frac{dt_1}{t_1}\int_0^{t_1}\frac{dt_2}{1-t_2} &= \int_0^1 \frac{dt_1}{t_1}\int_0^{t_1}\sum_{n=0}^{\infty} t_2^n dt_2 = \int_0^1 \frac{dt_1}{t_1}\left[\sum_{n=0}^{\infty}\frac{t_2^{n+1}}{n+1}\right]_0^{t_1}\\ &= \int_0^1 \sum_{n=0}^{\infty}\frac{t_1^n}{n+1}dt_1 = \left[\sum_{n=0}^{\infty}\frac{t_1^{n+1}}{(n+1)^2}\right]_0^1 = \sum_{m>0}\frac{1}{m^2} = \zeta(2)\,.\end{aligned} \tag{2.1}$$

With the same idea one can also show that we have (Exercise 6 i))

$$\zeta(2,3) = \int_0^1 \frac{dt_1}{t_1}\int_0^{t_1}\frac{dt_2}{1-t_2}\int_0^{t_2}\frac{dt_3}{t_3}\int_0^{t_3}\frac{dt_4}{t_4}\int_0^{t_4}\frac{dt_5}{1-t_5}\,. \tag{2.2}$$

In general we will see that an index $\mathbf{k}=(k_1,\dots,k_r)$ correspondonds to an iterated integral of length $\mathrm{wt}(\mathbf{k})$, where each k_j gives a block of k_j-1 integrals over $\frac{dt}{t}$ and one integral over $\frac{dt}{1-t}$. To prove these iterated integrals in general we will introduce multiple polylogarithms, which can be seen as a simultaneous generalization of the polylogarithm ($r=1$) and multiple zeta values ($z=1$).

Definition 2.1. *For $|z|<1$ and $\mathbf{k}=(k_1,\dots,k_r)\in\mathbb{Z}_{\geq 1}^r$ we define the* **multiple polylogarithm** *by*

$$\mathrm{Li}_{\mathbf{k}}(z) = \mathrm{Li}_{k_1,\dots,k_r}(z) = \sum_{m_1>\dots>m_r>0}\frac{z^{m_1}}{m_1^{k_1}\cdots m_r^{k_r}}$$

and set $\mathrm{Li}_{\emptyset}(z)=1$.

For an arbitrary index $\mathbf{k}$ the $\mathrm{Li}_{\mathbf{k}}(z)$ are holomorphic functions in the open unit disc, but clearly when $\mathbf{k}$ is admissible $\mathrm{Li}_{\mathbf{k}}(z)$ is also defined for $z=1$ and we have

$$\mathrm{Li}_{\mathbf{k}}(1) = \zeta(\mathbf{k})\,.$$

Multiple polylogarithms also have an iterated integral expression, and for example using the same calculation as in (2.1) we see for example that

$$\mathrm{Li}_2(z) = \int_0^z \frac{dt_1}{t_1}\int_0^{t_1}\frac{dt_2}{1-t_2}\,.$$

It becomes clear that we will deal with iterated integrals of two different differential forms. To describe the iterated integrals and the shuffle product, we will therefore introduce the following algebraic setup.

2.1.1 The spaces $\mathfrak{H}$, $\mathfrak{H}^1$ and $\mathfrak{H}^0$

We denote by $\mathfrak{H} = \mathbb{Q}\langle x, y\rangle$ the polynomial ring in the the two non-commutative variables x and y. A monomial in x and y will also be called a **word**, and $\mathfrak{H}$ is therefore the $\mathbb{Q}$-vector space spanned by all words in the **letters** x and y. Further, we define the subspace $\mathfrak{H}^1 = \mathbb{Q} + \mathfrak{H}y$, which is spanned by the **empty word** 1 and all words in x and y which end in y. For $k \geq 1$ we define

$$z_k = x^{k-1}y\,.$$

With this we see that $\mathfrak{H}^1 = \mathbb{Q}\langle z_1, z_2, \dots\rangle$, i.e. we could say that $\mathfrak{H}^1$ is spanned by all words in the letters z_k. For an index $\mathbf{k} = (k_1, \dots, k_r) \in \mathbb{Z}^r_{\geq 1}$ we define

$$z_{\mathbf{k}} = z_{k_1} z_{k_2} \cdots z_{k_r} \in \mathfrak{H}^1$$

and set $z_\emptyset = 1$. Now define the space $\mathfrak{H}^0 = \mathbb{Q} + x\mathfrak{H}y$, which is the subspace of $\mathfrak{H}^1$ generated by all words which start in x and end in y. In other words, $\mathfrak{H}^0$ is spanned by all $z_{\mathbf{k}}$ with admissible indices $\mathbf{k}$. Summarizing everything we have

$$\mathfrak{H}^0 = \langle z_{\mathbf{k}} \mid \mathbf{k} \text{ admissible index}\rangle_{\mathbb{Q}} \quad \subset \quad \mathfrak{H}^1 = \langle z_{\mathbf{k}} \mid \mathbf{k} \text{ index}\rangle_{\mathbb{Q}} \quad \subset \quad \mathfrak{H} = \mathbb{Q}\langle x, y\rangle\,.$$

2.1.2 Iterated integral expression for Li and ζ

From now on we will restrict to real $|z| < 1$ and consider integrals on the real axis. Since $\mathrm{Li}_{\mathbf{k}}(z)$ is defined for any $\mathbf{k}$, we can view Li as a $\mathbb{Q}$-linear map from $\mathfrak{H}^1$ to the space of real valued continuous functions on $(0,1)$, i.e. $C((0,1);\mathbb{R})$, defined on the generators by

$$\begin{aligned} \mathrm{Li}\colon \mathfrak{H}^1 &\longrightarrow C((0,1);\mathbb{R}) \\ z_{\mathbf{k}} &\longmapsto \mathrm{Li}_{\mathbf{k}}(z)\,. \end{aligned} \tag{2.3}$$

By abuse of notation we write $\mathrm{Li}\colon w \mapsto \mathrm{Li}_w(z)$ for any $w \in \mathfrak{H}^1$, which is defined by linearly extending the definition on the generators $z_{\mathbf{k}}$. For example for $w = xyxxy + 2xxxxy = z_2z_3 + 2z_5 \in \mathfrak{H}^1$ we have $\mathrm{Li}_w(z) = \mathrm{Li}_{2,3}(z) + 2\,\mathrm{Li}_5(z)$. Now we want to describe the iterated integral expression for the multiple polylogarithm using this setup.

Lemma 2.2. *Let $w \in \mathfrak{H}^1$ be a linear combination of words all starting with the letter $a \in \{x, y\}$, i.e. $w = au$ for some $u \in \mathfrak{H}^1$. Then we have*

$$\frac{d}{dz}\,\mathrm{Li}_w(z) = \frac{d}{dz}\,\mathrm{Li}_{au}(z) = \begin{cases} \frac{1}{z}\,\mathrm{Li}_u(z)\,, & a = x \\ \frac{1}{1-z}\,\mathrm{Li}_u(z)\,, & a = y \end{cases}.$$

Proof. Since Li is linear it suffices to proof the statement for a word w. Assuming $w = z_{\mathbf{k}}$ for $\mathbf{k} = (k_1, \dots, k_r)$, we have

$$\frac{d}{dz}\,\mathrm{Li}_w(z) = \frac{d}{dz}\,\mathrm{Li}_{\mathbf{k}}(z) = \frac{d}{dz} \sum_{m_1 > \cdots > m_r > 0} \frac{z^{m_1}}{m_1^{k_1} m_2^{k_2} \cdots m_r^{k_r}} = \sum_{m_1 > \cdots > m_r > 0} \frac{z^{m_1 - 1}}{m_1^{k_1 - 1} m_2^{k_2} \cdots m_r^{k_r}}\,.$$

Let $a = x$, which is equivalent to $k_1 > 1$. In this case we obtain

$$\frac{d}{dz}\,\mathrm{Li}_w(z) = \frac{d}{dz}\,\mathrm{Li}_{xu}(z) = \frac{1}{z} \sum_{m_1 > \cdots > m_r > 0} \frac{z^{m_1}}{m_1^{k_1 - 1} m_2^{k_2} \cdots m_r^{k_r}} = \frac{1}{z}\,\mathrm{Li}_u(z)\,.$$

If $a = y$, then we have $k_1 = 1$ and

$$\begin{aligned}\frac{d}{dz}\operatorname{Li}_w(z) = \frac{d}{dz}\operatorname{Li}_{yu}(z) &= \sum_{m_1>\cdots>m_r>0} \frac{z^{m_1-1}}{m_2^{k_2}\cdots m_r^{k_r}} = \sum_{m_2>\cdots>m_r>0} \frac{1}{m_2^{k_2}\cdots m_r^{k_r}} \sum_{m_1=m_2+1}^{\infty} z^{m_1-1} \\ &= \frac{1}{1-z} \sum_{m_2>\cdots>m_r>0} \frac{z^{m_2}}{m_2^{k_2}\cdots m_r^{k_r}} = \frac{1}{1-z}\operatorname{Li}_{k_2,\dots,k_r}(z) = \frac{1}{1-z}\operatorname{Li}_u(z)\,.\end{aligned}$$

□

Motivated by the iterated integrals (2.1), (2.2), and the above Lemma, we define

$$\omega_x(t) = \frac{dt}{t}\,, \qquad \omega_y(t) = \frac{dt}{1-t}\,.$$

With these differential forms we can write the multiple polylogarithms as the following iterated integral.

Proposition 2.3. *For any word $w = a_1 \dots a_k \in \mathfrak{H}^1$, with $a_1, \dots, a_k \in \{x, y\}$ and $0 \le z < 1$ we have*

$$\operatorname{Li}_w(z) = \int_0^z \omega_{a_1}(t_1) \int_0^{t_1} \omega_{a_2}(t_2) \cdots \int_0^{t_{k-1}} \omega_{a_k}(t_k)\,.$$

Proof. This follows from Lemma 2.2 by induction on k. In the case $k = 1$ we have $w = y = z_1$, i.e.

$$\operatorname{Li}_w(z) = \operatorname{Li}_1(z) = \sum_{m>0} \frac{z^m}{m} = \int_0^z \frac{dt}{1-t} = \int_0^z \omega_y(t)\,. \tag{2.4}$$

The induction step is then exactly the statement of Lemma 2.2 since $\operatorname{Li}_w(0) = 0$ for non-empty w. □

For a real z we will also use the following simplified notation for iterated integrals for $a_1 \dots a_k \in \mathfrak{H}^1$

$$\int_{z>t_1>\cdots>t_k>0} \omega_{a_1}(t_1)\cdots\omega_{a_k}(t_k) := \int_0^z \omega_{a_1}(t_1) \int_0^{t_1} \omega_{a_2}(t_2) \cdots \int_0^{t_{k-1}} \omega_{a_k}(t_k)\,.$$

Since $\zeta(\mathbf{k})$ is just defined for admissible indices, we can, similar to (2.3), define a $\mathbb{Q}$-linear map from $\mathfrak{H}^0$ to the space of multiple zeta values $\mathcal{Z}$, defined on the generators by

$$\begin{aligned}\zeta\colon \mathfrak{H}^0 &\longrightarrow \mathcal{Z} \\ z_{\mathbf{k}} &\longmapsto \zeta(\mathbf{k})\,.\end{aligned} \tag{2.5}$$

Also here we write $\zeta\colon w \mapsto \zeta(w)$ for any $w \in \mathfrak{H}^0$. Since $\operatorname{Li}_w(1) = \zeta(w)$ for any $w \in \mathfrak{H}^0$ we also get an iterated integral expression for multiple zeta values as a consequence of Proposition 2.3.

Corollary 2.4. *For any word $w = a_1 \dots a_k \in \mathfrak{H}^0$, with $a_1, \dots, a_k \in \{x, y\}$ we have*

$$\zeta(w) = \int_{1>t_1>\cdots>t_k>0} \omega_{a_1}(t_1)\cdots\omega_{a_k}(t_k)\,.$$

2.1.3 Duality relation

We now give a direct consequence of the iterated integral expression. Making the change of variables $s_j = 1 - t_{k-j+1}$ in the iterated integral expression gives a linear relation among multiple zeta values, which is called the duality relation. For example if $k = 3$ we can make the change of variables $s_1 = 1 - t_3$, $s_2 = 1 - t_2$, $s_3 = 1 - t_1$ in the following iterated integral

$$\begin{aligned}\zeta(3) = \int_0^1 \frac{dt_1}{t_1} \int_0^{t_1} \frac{dt_2}{t_2} \int_0^{t_2} \frac{dt_3}{1-t_3} &= \int_1^0 \frac{-ds_3}{1-s_3} \int_1^{s_3} \frac{-ds_2}{1-s_2} \int_1^{s_2} \frac{-ds_1}{s_1} \\ &= \int_0^1 \frac{ds_1}{s_1} \int_0^{s_1} \frac{ds_2}{1-s_2} \int_0^{s_2} \frac{ds_3}{1-s_3} = \zeta(2,1)\,.\end{aligned} \tag{2.6}$$

from which we again get the relation $\zeta(3) = \zeta(2,1)$ in Proposition 1.8. This change of variables can be described nicely in terms of an anti-automorphism on the space $\mathfrak{H}$. For this we denote by τ the anti-automorphism of $\mathfrak{H}$ which interchanges x and y. Here we view $\mathfrak{H}$, and all its subspaces, as $\mathbb{Q}$-algebras where the product is given by the usual non-commutative product in $\mathbb{Q}\langle x,y\rangle$. That τ is an anti-automorphism just means that $\tau(uw) = \tau(w)\tau(u)$ for $u, w \in \mathfrak{H}$ and $\tau(1) = 1$. For example if $w = z_3 = xxy$, then

$$\tau(z_3) = \tau(xxy) = \tau(y)\tau(xx) = \tau(y)\tau(x)\tau(x) = xyy = z_2 z_1\,.$$

Notice that $\tau(\mathfrak{H}^0) \subset \mathfrak{H}^0$, since any non-empty word $w \in \mathfrak{H}^0$ is of the form $w = xuy$ for some $u \in \mathfrak{H}$ and therefore $\tau(w) = \tau(xuy) = \tau(y)\tau(u)\tau(x) = x\tau(u)y \in \mathfrak{H}^0$. Further notice that τ is an involution, i.e. $\tau^2 = \mathrm{id}_{\mathfrak{H}}$ and $\tau(\mathfrak{H}^0) = \mathfrak{H}^0$.

Proposition 2.5 (Duality relation)**.** *For all $w \in \mathfrak{H}^0$ we have*

$$\zeta(\tau(w)) = \zeta(w)\,.$$

Proof. This is just a generalization of the variable change $s_j = 1 - t_{k-j+1}$ in the iterated integral expression in Corollary 2.4 similar to (2.6). Interchanging x and y corresponds to $\omega_a(t_{k-j+1}) = -\omega_{\tau(a)}(1-s_j)$ for $a \in \{x,y\}$. The property of τ being an anti-automorphism corresponds to changing the order/directions of the integrals, which also gets rid of the minus signs. □

A few explicit examples of the duality relations are given by the following Corollary, which both can be seen as a generalization of the formula $\zeta(3) = \zeta(2,1)$. Here we use the common notation $\{k_1,\dots,k_r\}^n = \underbrace{k_1,\dots,k_r \dots k_1,\dots,k_r}_{rn}$ for n copies of the string $k_1,\dots,k_r$.

Corollary 2.6. *i) For all $k \geq 3$ we have*

$$\zeta(k) = \zeta(2,\underbrace{1,\dots,1}_{k-2}) = \zeta(2,\{1\}^{k-2})\,.$$

ii) For all $n \geq 1$ we have

$$\zeta(\{2,1\}^n) = \zeta(\{3\}^n)\,.$$

Proof. Both statements are immediate consequences of the duality relations, since $\tau(z_k) = \tau(x^{k-1}y) = xy^{k-1} = z_2 z_1 \cdots z_1$ and $\tau((z_2z_1)^n) = \tau(z_2z_1)^n = z_3^n$. □

Remark 2.7. In Section 3 we will see another proof of the duality relation, which is not using the iterated integral expression. This new proof is based on so-called connected sums, which were just recently introduced by Seki and Yamamoto in [SY]. There we will also see that the duality is true for the q-analogue model of Bradley-Zhao (3.7) and that we we have $\zeta_q^{\mathrm{BZ}}(\tau(w)) = \zeta_q^{\mathrm{BZ}}(w)$, when considering ζ_q^{BZ} as a map from $\mathfrak{H}^1$ to $\mathbb{Q}[[q]]$.

2.2 The shuffle & stuffle product and finite double shuffle relations

In this subsection we will introduce the shuffle product $ш$ and stuffle product $*$ on the spaces $\mathfrak{H}$, $\mathfrak{H}^1$ and $\mathfrak{H}^0$. We will then show that the space $\mathcal{Z}$ is a $\mathbb{Q}$-algebra (i.e. give a proof of Proposition 1.11) and see that the map ζ in (2.5) is an algebra homomorphism from $\mathfrak{H}^0$ to $\mathbb{R}$ with respect to both products $ш$ and $*$. This will then lead to families of linear relations, which are called finite double shuffle relations.

2.2.1 The shuffle product

The iterated integral expressions give another way to obtain the shuffle product formula

$$\zeta(k_1)\zeta(k_2) = \sum_{j=2}^{k_1+k_2-1} \left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1} \right) \zeta(j, k_1+k_2-j)$$

in Proposition 1.9, which was proved by using partial fraction decomposition. For example we have

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

We will now describe how this relation can also be obtained from the iterated integral expression in Corollary 2.4. Using the iterated integral expression of $\zeta(2)$ and $\zeta(3)$ we get

$$\zeta(2)\zeta(3) = \int\limits_{1>t_1>t_2>0} \omega_x(t_1)\omega_y(t_2) \int\limits_{1>s_1>s_2>s_3>0} \omega_x(s_1)\omega_x(s_2)\omega_y(s_3)\,.$$

By blue we indicate the variables which correspond to the differential form ω_x and by red the ones corresponding to ω_y. This makes it easier to translate the iterated integrals below back to multiple zeta values. Using Fubini's theorem the right-hand side is the iterated integral of $\omega_x(t_1)\omega_y(t_2)\omega_x(s_1)\omega_x(s_2)\omega_y(s_3)$ over the domain where $1 > t_1 > t_2 > 0$ and $1 > s_1 > s_2 > s_3 > 0$. This can be decomposed into the following iterated integrals, where we can neglect the non-trivial intersections $t_j = s_i$ since they have measure zero.

$$\begin{aligned}
\zeta(2)\zeta(3) = \Bigg(&\int\limits_{1>t_1>t_2>s_1>s_2>s_3>0} + \int\limits_{1>t_1>s_1>t_2>s_2>s_3>0} + \int\limits_{1>s_1>t_1>t_2>s_2>s_3>0} + \int\limits_{1>s_1>t_1>s_2>t_2>s_3>0} \\
&+ \int\limits_{1>s_1>s_2>t_1>t_2>s_3>0} + \int\limits_{1>s_1>s_2>t_1>s_3>t_2>0} + \int\limits_{1>s_1>s_2>s_3>t_1>t_2>0} + \int\limits_{1>t_1>s_1>s_2>t_2>s_3>0} \\
&+ \int\limits_{1>t_1>s_1>s_2>s_3>t_2>0} + \int\limits_{1>s_1>t_1>s_2>s_3>t_2>0} \Bigg) \omega_x(t_1)\omega_y(t_2)\omega_x(s_1)\omega_x(s_2)\omega_y(s_3) \\
&= \zeta(2,3) + \zeta(3,2) + \zeta(3,2) + \zeta(4,1) + \zeta(4,1) + \zeta(4,1) + \zeta(3,2) + \zeta(4,1) + \zeta(4,1) + \zeta(4,1) \\
&= \zeta(2,3) + 3\zeta(3,2) + 6\zeta(4,1)\,.
\end{aligned}$$

The above example shows the origin of the name shuffle product, since one can interpret a multiple zeta value as a deck of blue and red cards, which correspond to the differential forms ω_x and ω_y. Taking the product of two multiple zeta values then corresponds just to the shuffle of these two decks of cards. We will now describe this product on the space $\mathfrak{H}$ and its subspaces.

Definition 2.8. *We define the* **shuffle product** $ш$ *on* $\mathfrak{H}$ *as the* $\mathbb{Q}$*-bilinear product, which satisfies* $1 ш w = w ш 1 = w$ *for any word* $w \in \mathfrak{H}$ *and*

$$a_1 w_1 ш a_2 w_2 = a_1(w_1 ш a_2 w_2) + a_2(a_1 w_1 ш w_2)$$

for any letters $a_1, a_2 \in \{x, y\}$ *and words* $w_1, w_2 \in \mathfrak{H}$.

By induction on the lengths of words, one can show that $ш$ is a commutative and associative product and $\mathfrak{H}_ш = (\mathfrak{H}, ш)$ is therefore a commutative $\mathbb{Q}$-algebra. One can also see that the subspaces $\mathfrak{H}^1$ and $\mathfrak{H}^0$ are both closed under $ш$ and therefore we have subalgebras $\mathfrak{H}^0_ш \subset \mathfrak{H}^1_ш \subset \mathfrak{H}_ш$. You can check that this definition corresponds exaclty to multiplying iterated integrals as above, i.e. we have

$$z_2 ш z_3 = xy ш xxy = xyxxy + 3xxyxy + 6xxxyy = z_2 z_3 + 3 z_3 z_2 + 6 z_4 z_1 \,.$$

That this is true in general will be proven now.

Proposition 2.9. *For any* $w, u \in \mathfrak{H}^1$ *we have*

$$\mathrm{Li}_w(z) \, \mathrm{Li}_u(z) = \mathrm{Li}_{w ш u}(z) \,,$$

i.e. the map Li *is an algebra homomorphism from* $\mathfrak{H}^1_ш$ *to* $C((0,1);\mathbb{R})$.

Proof. It is sufficient to prove the statement for words $w, u \in \mathfrak{H}^1$. We will do this by induction on the sum of the lengths of w and u. If one of them equals the empty word 1, the statement is clear. So lets assume that $w = aw'$ and $u = bu'$ for words $w', u' \in \mathfrak{H}^1$ and letters $a, b \in \{x, y\}$. Then we have

$$\frac{d}{dz}\left(\mathrm{Li}_w(z)\,\mathrm{Li}_u(z)\right) = \frac{d}{dz}\left(\mathrm{Li}_{aw'}(z)\,\mathrm{Li}_{bu'}(z)\right) = \left(\frac{d}{dz}\mathrm{Li}_{aw'}(z)\right)\mathrm{Li}_{bu'}(z) + \mathrm{Li}_{aw'}(z)\left(\frac{d}{dz}\mathrm{Li}_{bu'}(z)\right) .$$

Using now Lemma 2.2 we get $\frac{d}{dz}\mathrm{Li}_{aw'}(z) = f_a(z)\,\mathrm{Li}_{w'}(z)$ with $f_x(z) = \frac{1}{z}$ and $f_y(z) = \frac{1}{1-z}$. Using this together with the induction hypothesis we have

$$\frac{d}{dz}\left(\mathrm{Li}_w(z)\,\mathrm{Li}_u(z)\right) = f_a(z)\,\mathrm{Li}_{w'}(z)\,\mathrm{Li}_{bu'}(z) + f_b(z)\,\mathrm{Li}_{aw'}(z)\,\mathrm{Li}_{u'}(z) = f_a(z)\,\mathrm{Li}_{w' ш bu'}(z) + f_b(z)\,\mathrm{Li}_{aw' ш u'}(z) .$$

Applying Lemma 2.2 again gives

$$\frac{d}{dz}\left(\mathrm{Li}_w(z)\,\mathrm{Li}_u(z)\right) = \frac{d}{dz}\mathrm{Li}_{a(w' ш bu')}(z) + \frac{d}{dz}\mathrm{Li}_{b(aw' ш u')}(z) = \frac{d}{dz}\mathrm{Li}_{w ш u}(z) \,,$$

i.e. $\mathrm{Li}_w(z)\,\mathrm{Li}_u(z) = \mathrm{Li}_{w ш u}(z) + c$ for some constant c. But since both sides vanish for $z = 0$, we conclude $c = 0$. ☐

For $w, u \in \mathfrak{H}^0$ we can also set $z = 1$ in the Proposition above and obtain the following.

Corollary 2.10. *For any* $w, u \in \mathfrak{H}^0$ *we have*

$$\zeta(w)\zeta(v) = \zeta(w ш v) \,.$$

In particular the space $\mathcal{Z}$ *is a* $\mathbb{Q}$*-subalgebra of* $\mathbb{R}$ *and* ζ *is an algebra homomorphism from* $\mathfrak{H}^0_ш$ *to* $\mathcal{Z}$.

2.2.2 The stuffle product

In Section 1 we saw that for $k_1, k_2 \geq 2$ we have the stuffle product formula

$$\zeta(k_1)\zeta(k_2) = \left(\sum_{m_1 > m_2 > 0} + \sum_{m_2 > m_1 > 0} + \sum_{m_1 = m_2 > 0} \right) \frac{1}{m_1^{k_1} m_2^{k_2}} = \zeta(k_1, k_2) + \zeta(k_2, k_1) + \zeta(k_1 + k_2)\,.$$

With the same argument, i.e. splitting up the summation, we get for $k_1, k_2 \geq 2$, $k_3 \geq 1$

$$\zeta(k_1)\zeta(k_2, k_3) = \zeta(k_1, k_2, k_3) + \zeta(k_2, k_1, k_3) + \zeta(k_2, k_3, k_1) + \zeta(k_1 + k_2, k_3) + \zeta(k_2, k_1 + k_3)\,.$$

Similar to the shuffle product we will now define the stuffle product $*$ on the space $\mathfrak{H}^1$ and $\mathfrak{H}^0$ and then show that ζ is also an algebra homomorphism with respect to this product. Recall that $\mathfrak{H}^1 = \mathbb{Q}\langle z_1, z_2, \dots \rangle$, i.e. every element in $\mathfrak{H}^1$ can be viewed as a linear combination of words in the letters z_j instead of the letters x, y. Here and in the following we will use the terminology 'word' in these two different ways and it will be clear from context if we talk about words in the z_j or x, y. In the next subsection we will see that the shuffle and the shuffle product are both examples of quasi-shuffle products over different alphabets.

Definition 2.11. *We define the* **stuffle product** $*$ *on* $\mathfrak{H}^1$ *as the* $\mathbb{Q}$*-bilinear product, which satisfies* $1 * w = w * 1 = w$ *for any word* $w \in \mathfrak{H}^1$ *and*

$$z_i w_1 * z_j w_2 = z_i(w_1 * z_j w_2) + z_j(z_i w_1 * w_2) + z_{i+j}(w_1 * w_2)$$

for any $i, j \geq 1$ *and words* $w_1, w_2 \in \mathfrak{H}^1$.

Notice that this product also replicated the above product formula of multiple zeta values, since

$$z_{k_1} * z_{k_2} = z_{k_1} z_{k_2} + z_{k_2} z_{k_1} + z_{k_1 + k_2}\,.$$

This product is also called the harmonic product and one can check (see [H1]) that it is commutative and associate and therefore $\mathfrak{H}^1_* = (\mathfrak{H}^1, *)$ is a commutative $\mathbb{Q}$-algebra. By definition it is easy to check that $\mathfrak{H}^0$ is also closed under $*$ and we get a subalgebra $\mathfrak{H}^0_* \subset \mathfrak{H}^1$.
In the case of the shuffle product we used the polylogarithm to prove that the product of multiple zeta values satisfy the shuffle product formula by consdering $z = 1$. In the case of the stuffle product, we will consider the **truncated multiple zeta values** (also often called multiple harmonic sums), which are for an integer $M \geq 1$ and any index $\mathbf{k} = (k_1, \dots, k_r) \in \mathbb{Z}^r_{\geq 1}$ defined by

$$\zeta_M(\mathbf{k}) = \zeta_M(k_1, \dots, k_r) = \sum_{M > m_1 > \dots > m_r > 0} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}} \in \mathbb{Q}\,.$$

Clearly if $\mathbf{k}$ is admissible we have $\lim_{M \to \infty} \zeta_M(\mathbf{k}) = \zeta(\mathbf{k})$. For a fixed M we can view ζ_M as a $\mathbb{Q}$-linear map from $\mathfrak{H}^1$ to $\mathbb{Q}$, defined on the generators by $\zeta_M \colon z_{\mathbf{k}} \mapsto \zeta_M(\mathbf{k})$.

Proposition 2.12. *For any* $w, u \in \mathfrak{H}^1$ *and* $M \geq 1$ *we have*

$$\zeta_M(w)\zeta_M(u) = \zeta_M(w * u)\,,$$

i.e. the map ζ_M *is an algebra homomorphism from* $\mathfrak{H}^1_*$ *to* $\mathbb{Q}$.

Proof. This can be done by induction on the depths or M (Exercise 6 ii). We will prove this in more general form for quasi-shuffle algebras in the next section (Lemma 2.18). □

For $w, u \in \mathfrak{H}^0$ we can also take the limit $M \to \infty$ in the Proposition above and obtain the following.

Corollary 2.13. *For any* $w, u \in \mathfrak{H}^0$ *we have*

$$\zeta(w)\zeta(v) = \zeta(w * v)\,,$$

i.e. ζ *is an algebra homomorphism from* $\mathfrak{H}^0_*$ *to* $\mathcal{Z}$.

2.2.3 Finite double shuffle relations

Since the map $\zeta\colon \mathfrak{H}^0 \to \mathcal{Z}$ is an algebra homomorphism with respect to the shuffle product $\sqcup\!\sqcup$ and the stuffle product $*$, we get a large family of linear relations among multiple zeta values.

Proposition 2.14 (Finite double shuffle relations)**.** *For $w, u \in \mathfrak{H}^0$ we have*

$$\zeta(w \sqcup\!\sqcup u - w * u) = 0\,.$$

But it is also clear, that these do not give all linear relations among multiple zeta values. For example the relation $\zeta(3) = \zeta(2,1)$ is not a consequence of the above Proposition. Counting the finite double shuffle relations, we get the following table, which comes from the survey article [Tan]. In this article, you can also find the numbers of other families of relations, such as the duality relation.

weight k	3	4	5	6	7	8	9	10	11	12
# all conjectured relations	1	3	6	14	29	60	123	249	503	1012
# finite double shuffle relations	0	1	2	7	16	40	92	200	429	902

We see that the first possible finite double shuffle relation appears in weight 4 by choosing $w = u = z_2$, which gives

$$w \sqcup\!\sqcup u - w * u = (2z_2z_2 + 4z_3z_1) - (2z_2z_2 + z_4) = 4z_3z_1 - z_4$$

i.e. $4\zeta(3,1) = \zeta(4)$. This relation is a special case of the following family of linear relations which is a consequence of finite double shuffle relations.

Proposition 2.15. *For all $n \geq 1$ we have*

$$4^n\zeta(\{3,1\}^n) = \zeta(\{4\}^n)\,.$$

Proof. This can be done by proving the following equations in $\mathfrak{H}^0$ (Exercise 7)

$$\sum_{j=-n}^{n} (-1)^j z_2^{n-j} \sqcup\!\sqcup z_2^{n+j} = 4^n(z_3z_1)^n\,, \qquad \sum_{j=-n}^{n} (-1)^j z_2^{n-j} * z_2^{n+j} = z_4^n\,.$$

(Notice: Here z_k^n means $z_kz_k\dots z_k$, i.e. the usual non-commutative product in $\mathfrak{H}$ and <u>not</u> the shuffle or stuffle product.) □

Together with the explicit formula (Exercise 7)

$$\zeta(\{2\}^n) = \frac{\pi^{2n}}{(2n+1)!} \tag{2.7}$$

the proof of Proposition 2.15 can also be used to show

$$\zeta(\{4\}^n) = \frac{4^n 2\pi^{4n}}{(4n+2)!}\,, \qquad \zeta(\{3,1\}^n) = \frac{2\pi^{4n}}{(4n+2)!}\,,$$

where the second equation here is known as the 3-1 formula for multiple zeta values.

2.3 Quasi-shuffle algebras

In this section, we want to generalize what we did in the previous section. On $\mathfrak{H}$, we defined the shuffle product on words in letters x and y, and on $\mathfrak{H}^1$, we defined the stuffle product on words in letters z_j for $j \geq 1$. This idea will be generalized now by allowing an arbitrary set of letters A and then define a product on the space of words in these letters. We will mainly follow the definitions and theorems in [HI] and [IKZ], but will also introduce some definitions and theorems, which can not be found in the literature.

2.3.1 The algebra of letters and words

In the following, we assume that k is a field containing $\mathbb{Q}$, and A is a countable set to which we refer as the **set of letters**. Let kA be the k-vector space generated by A and let $\diamond$ be a k-bilinear, associative and commutative product on kA. We obtain a (non-unital) k-algebra $(kA, \diamond)$, to which we refer as the **algebra of letters**. Notice that in the work [HI] the authors just assume that $\diamond$ is associative and commutative and do not consider kA as an algebra, but it will be useful for our purposes (e.g., Lemma 2.18). For such a product $\diamond$ on letters, we want to assign a product $*_\diamond$ on the space of words $k\langle A\rangle$, which generalizes the stuffle and shuffle product we have seen before. Here a monomial $w = a_1 \cdots a_l$ in $k\langle A\rangle = k\langle a_1, a_2, \dots\rangle$ will again be called a **word** and the unit ($l = 0$), denoted by 1, is again called the **empty word**. By $\ell(w) = l$ we denote the **length of the word** w.

Definition 2.16. *Let $\diamond$ be a product on kA as above. Then we define the* **quasi-shuffle product** $*_\diamond$ *on $k\langle A\rangle$ as the k-bilinear product, which satisfies $1 *_\diamond w = w *_\diamond 1 = w$ for any word $w \in k\langle A\rangle$ and*

$$aw *_\diamond bv = a(w *_\diamond bv) + b(aw *_\diamond v) + (a \diamond b)(w *_\diamond v) \tag{2.8}$$

for any letters $a, b \in A$ and words $w, v \in k\langle A\rangle$.

Theorem 2.17. *The space $k\langle A\rangle$ equipped with the product $*_\diamond$ becomes a commutative k-algebra.*

Proof. This is Theorem 2.1 in [HI]. It suffices to show that $*_\diamond$ is commutative and associative, which can be done straightforward by induction on the lengths of words. □

We will call $(k\langle A\rangle, *_\diamond)$ a **quasi-shuffle algebra** or **algebra of words**. Notice that this generalized the $\mathbb{Q}$-algebra $\mathfrak{H}_{ш}$ by choosing $k = \mathbb{Q}$, $A = \{x, y\}$ and $a \diamond b = 0$ for any letters $\{x, y\}$ and it generalizes the $\mathbb{Q}$-algebra $\mathfrak{H}^1_*$, by choosing $k = \mathbb{Q}$, $A = \{z_1, z_2, \dots\}$ and $z_i \diamond z_j = z_{i+j}$ (See section 2.3.2 for details). Our purpose to introduce quasi-shuffle products is to also describe the product structure of the q-series $\mathrm{g}(\mathbf{k})$ and the (modified) q-analogues ζ_q.

Lemma 2.18. *Let R be a k-algebra and $f_m \colon (kA, \diamond) \to R$ be k-algebra homomorphisms for $m \geq 1$. Then for all $M \geq 1$ the k-linear map $F_M : k\langle A\rangle \to R$ defined on a word $w = a_1 \cdots a_r \in k\langle A\rangle$ by*

$$F_M(w) = \sum_{M > m_1 > \cdots > m_r > 0} f_{m_1}(a_1) \cdots f_{m_r}(a_r)$$

and $F_M(1) = 1$ is a k-algebra homomorphism from $(k\langle A\rangle, *_\diamond)$ to R.

Proof. It suffices to show that for any $M \geq 1$ and words $w, v \in k\langle A\rangle$ we have

$$F_M(w) F_M(v) = F_M(w *_\diamond v) .$$

We will prove this by induction on M. The case $M=1$ is trivial, since $F_1(w)=0$ for all non-empty w and $1=F_1(1)F_1(1)=F_1(1*_\diamond 1)$. Notice that we have $F_M(aw)=\sum_{M>m>0} f_m(a)F_m(w)$ for a letter a and a word w. For $w=aw'$, $v=bv'$ with letters $a,b\in A$ and words $w',v'\in k\langle A\rangle$ we therefore get

$$\begin{aligned}
F_M(w)F_M(v) &= \sum_{M>m>0} f_m(a)F_m(w') \sum_{M>n>0} f_n(b)F_n(v') \\
&= \left(\sum_{M>m>n>0} + \sum_{M>n>m>0} + \sum_{M>m=n>0} \right) f_m(a)F_m(w')f_n(b)F_n(v') \\
&= \sum_{M>m>0} f_m(a)F_m(w')F_m(bv') + \sum_{M>n>0} f_n(b)F_n(aw')F_n(v') + \sum_{M>m>0} f_m(a)f_m(b)F_m(w')F_m(v') \\
&= \sum_{M>m>0} f_m(a)F_m(w' *_\diamond bv') + \sum_{M>n>0} f_n(b)F_n(aw' *_\diamond v') + \sum_{M>m>0} f_m(a\diamond b)F_m(w' *_\diamond v') \\
&= F_M(a(w' *_\diamond bv')) + F_M(b(aw' *_\diamond v')) + F_M((a\diamond b)(w' *_\diamond v')) = F_M(w *_\diamond v)\,.
\end{aligned}$$

Here we used that f_m is an algebra homomorphism together with the induction hypothesis in the fourth equation. □

2.3.2 Examples of quasi-shuffle products & (sub)algebras

In the following, we give a few explicit examples for quasi-shuffle products and algebras which appear in this course. We will also consider certain subalgebras, and the first statement we want to show now is that subalgebras of the algebra of letters gives subalgebras of the algebra of words.

Proposition 2.19. *If $B\subset A$ is a subset of letters such that $(kB,\diamond)$ is a subalgebra of $(kA,\diamond)$, then $(k\langle B\rangle, *_\diamond)$ is a subalgebra of $(k\langle A\rangle, *_\diamond)$.*

Proof. We need to show that $k\langle B\rangle$ is closed under $*_\diamond$. But this follows directly from the definition of $*_\diamond$, since if kB is closed under $\diamond$ then we have for $a,b\in B$ that $a\diamond b\in B$. Therefore all emenents on the right-hand side of (2.8) are in $k\langle B\rangle$ if $w,v\in k\langle B\rangle$ and $a,b\in B$. □

Most of our objects depend on some index $\mathbf{k}=(k_1,\dots,k_r)$ and therefore most of our examples use the set of letters, the "z-alphabet", defined by

$$A_z := \{z_1, z_2, \dots\}\,.$$

Notice that we have a abuse of notion here, since $z_k = x^{k-1}y$ denoted elements in $\mathfrak{H}$ previously. But from the context it should always be clear if we talk about the formal elements z_k in A_z or the elements in $\mathfrak{H}$.

i) **Shuffle product** For any field k and any set of letters A, one can define the trivial product $a\diamond b=0$ for $a,b\in A$. The resulting quasi-shuffle product is then just the shuffle product $ш = *_\diamond$. As a special case we considered $k=\mathbb{Q}$, $A=\{x,y\}$ before but will also deal with the shuffle product on A_z later, which is sometimes also called the "index-shuffle product".

ii) **Stuffle product** Another example we considered before is the stuffle product. Choosing $k=\mathbb{Q}$, $A_z=\{z_1,z_2,\dots\}$ and $z_i\diamond z_j = z_{i+j}$ we write $* = *_\diamond$. Here the z_j are considered as variables itself, but we see that $(\mathbb{Q}\langle A_z\rangle, *)$ is isomorphic to $\mathfrak{H}^1_*$ as a $\mathbb{Q}$-algebra, when sending z_k to $x^{k-1}y$. Notice that the algebra of letters $(\mathbb{Q}A_z,\diamond)$ is isomorphic to $X\mathbb{Q}[X]$, by sending z_k to X^k. Defining for $m\geq 1$ the algebra homomorphisms $f_m : X\mathbb{Q}[X]\to\mathbb{Q}$ by $p\mapsto p\left(m^{-1}\right)$ gives the truncated multiple zeta values ζ_M as the function F_M in Lemma 2.18. In particular we obtain Proposition 2.12 as a consequence. Considering the subsets $A_z^{\geq 2} \subset A_z$ and $A_z^{\mathrm{ev}} \subset A_z$ defined by

$$A_z^{\geq 2} := A_z \backslash \{z_1\} = \{z_2, z_3, z_4, \dots\}, \qquad A_z^{\mathrm{ev}} := \{z_2, z_4, z_6, \dots\},$$

we clearly have that $(\mathbb{Q}A_z^{\geq 2}, \diamond)$ and $(\mathbb{Q}A_z^{\mathrm{ev}}, \diamond)$ are subalgebras of $(\mathbb{Q}A_z, \diamond)$. As a consequence of Proposition 2.19 we see that

$$\mathcal{Z}^{\geq 2} = \left\langle \zeta(k_1, \dots, k_r) \mid r \geq 0,\, k_1, \dots, k_r \geq 2 \right\rangle_{\mathbb{Q}},$$
$$\mathcal{Z}^{\mathrm{ev}} = \left\langle \zeta(k_1, \dots, k_r) \mid r \geq 0,\, k_1, \dots, k_r \geq 2 \text{ even} \right\rangle_{\mathbb{Q}}$$

are subalgebras of $\mathcal{Z}$. Notice that by Browns Theorem 1.17 we actually have $\mathcal{Z}^{\geq 2} = \mathcal{Z}$.

iii) **The q-series $\mathrm{g}(\mathbf{k})$:** Recall that we defined for an index $\mathbf{k} = (k_1, \dots, k_r)$ the modified q-analogues

$$\mathrm{g}(\mathbf{k}) = \mathrm{g}(k_1, \dots, k_r) = \sum_{m_1 > \dots > m_r > 0} \frac{P_{k_1}(q^{m_1})}{(1-q^{m_1})^{k_1}} \cdots \frac{P_{k_r}(q^{m_r})}{(1-q^{m_r})^{k_r}} \in \mathbb{Q}[[q]].$$

Inspired by Lemma 1.28 we define on $\mathbb{Q}A_z$ the product

$$z_{k_1} \hat{\diamond} z_{k_2} = z_{k_1+k_2} + \sum_{j=1}^{k_1+k_2-1} \left(\lambda_{k_1,k_2}^j + \lambda_{k_2,k_1}^j \right) z_j \tag{2.9}$$

where the rational numbers λ_{k_1,k_2}^j are given by

$$\lambda_{k_1,k_2}^j = (-1)^{k_2-1} \binom{k_1+k_2-1-j}{k_1-j} \frac{B_{k_1+k_2-j}}{(k_1+k_2-j)!}.$$

It is easy to see that this product is indeed associative and commutative. By Lemma 1.28 we see that for $m \geq 1$ the map $f_m : \mathbb{Q}A_z \to \mathbb{Q}[[q]]$ defined on the generators by

$$f_m(z_k) = \frac{P_k(q^m)}{(1-q^m)^k}$$

is a $\mathbb{Q}$-algebra homomorphism from $(\mathbb{Q}A_z, \hat{\diamond})$ to $\mathbb{Q}[[q]]$. We will denote the corresponding quasi-shuffle product by $\hat{*} = *_{\hat{\diamond}}$. Using Lemma 2.18, we see that, after taking the limit $M \to \infty$, that the space $\mathcal{G}$, spanned by all $\mathrm{g}(\mathbf{k})$, is a $\mathbb{Q}$-subalgebra of $\mathbb{Q}[[q]]$ and we can view $\mathcal{G}$ as an algebra homomorphism from $(\mathbb{Q}\langle A_z \rangle, \hat{*})$ to $\mathcal{G}$. This proofs Proposition 1.27.

Proposition 2.20. *The subspaces $\mathcal{G}^{ev} \subset \mathcal{G}^{\geq 2} \subset \mathcal{G}$, defined by*

$$\mathcal{G}^{\geq 2} = \left\langle \mathrm{g}(k_1, \dots, k_r) \mid r \geq 0,\, k_1, \dots, k_r \geq 2 \right\rangle_{\mathbb{Q}},$$
$$\mathcal{G}^{ev} = \left\langle \mathrm{g}(k_1, \dots, k_r) \mid r \geq 0,\, k_1, \dots, k_r \geq 2 \textit{ even} \right\rangle_{\mathbb{Q}},$$

are $\mathbb{Q}$-subalgebras of $\mathcal{G}$.

Proof. This will be a consequence of Proposition 2.19 after showing that $(\mathbb{Q}A_z^{\geq 2}, \hat{\diamond})$ and $(\mathbb{Q}A_z^{\mathrm{ev}}, \hat{\diamond})$ are subalgebras of $(\mathbb{Q}A_z, \hat{\diamond})$. Assume $z_{k_1}, z_{k_2} \in A_z^{\geq 2}$, i.e. $k_1, k_2 \geq 2$, then we see that all elements on the right-hand side in (2.9) are in $\mathbb{Q}A_z^{\geq 2}$, since $\lambda^1_{k_1,k_2} + \lambda^1_{k_2,k_1} = 0$ in these cases. This can be seen by writing

$$\lambda^1_{k_1,k_2} + \lambda^1_{k_2,k_1} = \left((-1)^{k_1} + (-1)^{k_2}\right) \binom{k_1+k_2-2}{k_1-1} \frac{B_{k_1+k_2-1}}{(k_1+k_2-j)!} . \tag{2.10}$$

If k_1 and k_2 have different parity then this is clearly zero and if $k_1 + k_2 \geq 4$ is even, then $k_1+k_2-1 \geq 3$ is odd and therefore $B_{k_1+k_2-1}$ vanishes. This shows that $(\mathbb{Q}A_z^{\geq 2}, \hat{\diamond})$ is a subalgebra of $(\mathbb{Q}A_z, \hat{\diamond})$.

Now assume that $z_{k_1}, z_{k_2} \in A_z^{\mathrm{ev}}$, i.e. k_1, k_2 are even. Since $B_k = 0$ for odd $k > 1$ we have that $\lambda^j_{k_1,k_2} = \lambda^j_{k_2,k_1} = 0$ in the cases that j is odd and $1 \leq j < k_1+k_2-1$. But since $k_1, k_2 \geq 2$ we also have that $\lambda^{k_1+k_2-1}_{k_1,k_2} = \lambda^{k_1+k_2-1}_{k_2,k_1} = 0$. This shows that all elements on the right-hand side in (2.9) are in $\mathbb{Q}A_z^{\mathrm{ev}}$ from which we get that $(\mathbb{Q}A_z^{\mathrm{ev}}, \hat{\diamond})$ is a subalgebra of $(\mathbb{Q}A_z, \hat{\diamond})$. □

iv) **Bradley-Zhao q-MZV:**We defined for an admissible index $\mathbf{k} = (k_1, \dots, k_r)$

$$\zeta_q^{\mathrm{BZ}}(\mathbf{k}) = \zeta_q^{\mathrm{BZ}}(k_1, \dots, k_r) = \sum_{m_1 > \dots > m_r > 0} \frac{q^{(k_1-1)m_1} \cdots q^{(k_r-1)m_r}}{[m_1]_q^{k_1} \cdots [m_r]_q^{k_r}} . \tag{2.11}$$

Since we have for $m \geq 1$ and $k_1, k_2 \geq 2$

$$\frac{q^{(k_1-1)m}}{[m]_q^{k_1}} \frac{q^{(k_2-1)m}}{[m]_q^{k_2}} = \frac{q^{(k_1+k_2-1)m}}{[m]_q^{k_1+k_2}} + (1-q) \frac{q^{(k_1+k_2-2)m}}{[m]_q^{k_1+k_2-1}}$$

we choose $k = \mathbb{Q}(1-q)$ and define on kA_z the product

$$z_{k_1} \diamond z_{k_2} = z_{k_1+k_2} + (1-q) z_{k_1+k_2-1}.$$

As before we get a quasi-shuffle algebra $(k\langle A_z\rangle, *_\diamond)$ and for a $M \geq 1$ an algebra homormorphism F_M to $\mathbb{Q}[[q]]$ by sending $z_{k_1} \dots z_{k_r}$ to the truncated version $\zeta^{\mathrm{BZ}}_{q.M}(k_1, \dots, k_r)$ defined in the obvious way. Notice that one could also consider the modified version $\overline{\zeta}_q^{\mathrm{BZ}}(\mathbf{k}) := (1-q)^{-\operatorname{wt}(\mathbf{k})} \zeta_q^{\mathrm{BZ}}(\mathbf{k})$. With this one can choose again $k = \mathbb{Q}$ and use the product $z_{k_1} \diamond z_{k_2} = z_{k_1+k_2} + z_{k_1+k_2-1}$. The algebraic structure of these modified version are for example studied in [Tak].

v) **Generalized modified q-MZV:** Take $A_{z,Q} = \{ z_k^Q \mid k \geq 1, Q \in \mathbb{Q}[X], \deg(Q) \leq k \}$ and define

$$z_{k_1}^{Q_1} \diamond z_{k_2}^{Q_2} = z_{k_1+k_2}^{Q_1 \cdot Q_2} .$$

Then clearly $f_m : (\mathbb{Q}A_z, \diamond) \to \mathbb{Q}[[q]]$ given by $f_m(z_k^Q) = \frac{Q(q^m)}{(1-q^m)^k}$ is an $\mathbb{Q}$-algebra homomorphism. Again as a consequence of Lemma 1.28 we see that the space $\mathcal{Z}_q$ is a $\mathbb{Q}$-subalgebra of $\mathbb{Q}[[q]]$.

2.3.3 Words of repeating letters

In the following subsection, we want to state some standard facts on quasi-shuffle algebras, which were established in [HI], [H2], and [IKZ] (without using the notion of quasi-shuffle algebras). Some of these will be given without proofs and we refer the reader to the above references for details.

Let $f=\sum_{n=0}^{\infty} c_n T^n \in k[[T]]$ and $\bullet \in \{\diamond, *_\diamond\}$, then we define for $a\in A$

$$f_\bullet(aX)=\sum_{n=0}^{\infty} c_n \underbrace{a\bullet\cdots\bullet a}_{n} X^n = \sum_{n=0}^{\infty} c_n a^{\bullet n} X^n \in k\langle A\rangle[[X]]\,.$$

In other words $f_\bullet(aX)$ means, that we plug aX into the power series f, and then use the product $\bullet$ to evaluate the products of a in $(aX)^n$. Therefore it also makes sense to consider $f_\bullet(zX)$ for any $z\in kA[[X]]$ and then evaluate $(zX)^n$ as an element in $(k\langle A\rangle, *_\diamond)[[X]]$ or $(kA,\diamond)[[X]]$. This we will do in Proposition 2.21 below. Notice that we have two different products on $k\langle A\rangle$ given by the quasi-shuffle product $*_\diamond$ and given by the usual non-commutative multiplication. When calculating with elements in $k\langle A\rangle[[X]]$, we will always do it with respect to the usual non-commutative multiplication in $k\langle A\rangle$.

Proposition 2.21. *For all $z\in kA[[X]]$ we have*

$$\exp_{*_\diamond}(\log_\diamond(1+zX))=\frac{1}{1-zX}\,. \tag{2.12}$$

Proof. This is [HI, Corollary 5.1], but it will also be a consequence of Proposition 2.29 below. ☐

Asumme we have an algebra homormorphism $\varphi : (k\langle A\rangle, *_\diamond)\to R$ in some k-algebra R. Applying φ to (2.12) with $z=a\in A$ gives the following equation in $R[[X]]$

$$\exp\left(\sum_{n=1}^{\infty}(-1)^{n-1}\varphi(a^{\diamond n})\frac{X^n}{n}\right)=1+\sum_{n=1}^{\infty}\varphi(a^n)X^n. \tag{2.13}$$

In particular we have

$$\varphi(a^n)\in k\left[\varphi(a^{\diamond j})\mid 1\le j\le n\right]\,, \tag{2.14}$$

i.e. for $a\in A$ the $\varphi(a^n)=\varphi(aa\cdots a)$ is a polynomial in $\varphi(a^{\diamond j})$ with $1\le j\le n$.

Corollary 2.22. *i) For all $k,M\ge 1$ we have*

$$\exp\left(\sum_{n=1}^{\infty}(-1)^{n-1}\zeta_M(nk)\frac{X^n}{n}\right)=1+\sum_{n=1}^{\infty}\zeta_M(\{k\}^n)X^n$$

and therefore $\zeta_M(\{k\}^n)\in\mathbb{Q}[\zeta_M(jk)\mid 1\le j\le n]$ for all $n\ge 1$. In particular, for $k\ge 2$ these statements also hold by replacing ζ_M with ζ.

ii) For all $k,n\ge 1$ we have

$$\mathrm{g}(\{k\}^n)\in\mathbb{Q}[\mathrm{g}(j)\mid 1\le j\le kn]\,.$$

In addition if $k\ge 2$ is even, then $\mathrm{g}(\{k\}^n)\in\mathbb{Q}[\mathrm{g}(j)\mid 2\le j\le kn\,, j$ even$]$

Proof. Statement i) follows directly from (2.13) by using the algebra homomorphism $\zeta_M : (\mathbb{Q}\langle A_z\rangle, *)\to\mathbb{Q}$, $a=z_k$ and the fact that $z_k^{\diamond n}=z_{kn}$ if $z_i\diamond z_j=z_{i+j}$. For ii) we use the algebra homomorphism $\mathrm{g} : (\mathbb{Q}\langle A_z\rangle, \hat{*})\to\mathbb{Q}[[q]]$ together with (2.14). The second part of ii) follows since $\mathbb{Q}A_z^{\mathrm{ev}}$ is closed under $\hat\diamond$ as we saw in Proposition 2.20 and therefore $z_k^{\hat\diamond n}\in\mathbb{Q}A_z^{\mathrm{ev}}$ if k is even. ☐

2.3.4 Application: Quasi-modular forms

By Proposition 1.1 we know that for $m \geq 1$ we have $\zeta(2m) \in \mathbb{Q}\pi^{2m}$ and with Corollary 2.22 we get

$$\zeta(2m, \dots, 2m) \in \mathbb{Q}[\zeta(2)] = \mathbb{Q}[\pi^2]\,.$$

For example as we have already seen before, we have for all $n \geq 1$

$$\zeta(\{2\}^n) = \frac{\pi^{2n}}{(2n+1)!}\,, \qquad \zeta(\{4\}^n) = \frac{4^n 2\pi^{4n}}{(4n+2)!}\,.$$

A similar statement can also be shown for the q-series g and the q-analogon of $\mathbb{Q}[\zeta(2)]$ is given by the **ring of quasi-modular forms** (with rational coefficients), defined by

$$\widetilde{\mathcal{M}}^{\mathbb{Q}} := \mathbb{Q}[\mathrm{g}(2), \mathrm{g}(4), \mathrm{g}(6)]\,.$$

As an anlogon from Euler formula for $\zeta(2m)$ we get the following.

Theorem 2.23. *For all $m \geq 1$ we have $\mathrm{g}(2m) \in \widetilde{\mathcal{M}}^{\mathbb{Q}}$.*

Proof. We will proof this in Section 5 and also give an explicit formula similar to the one of Euler for $\zeta(2m)$ in terms of $\zeta(2)$. But with some work this also follows from Proposition 1.29 and 1.30 (Similar to Exercise 4). ☐

Corollary 2.24. *For all $m \geq 1$ we have*

$$\mathrm{g}(2m, \dots, 2m) \in \widetilde{\mathcal{M}}^{\mathbb{Q}}\,.$$

Proof. This now follows directly from Theorem 2.23 and Corollary 2.22 ii). ☐

Proposition 2.25. *i) The space $\widetilde{\mathcal{M}}^{\mathbb{Q}}$ is closed under $q\frac{d}{dq}$.*

ii) We have

$$\widetilde{\mathcal{M}}^{\mathbb{Q}} = \mathbb{Q}[\mathrm{g}(2), \mathrm{g}'(2), \mathrm{g}''(2)]\,.$$

where g' denotes the derivative with respect to $q\frac{d}{dq}$.

iii) Let $\mathbf{k} = (k_1, \dots, k_r)$ be an index with $k_1, \dots, k_r \geq 2$ even. Then we have

$$\mathrm{g}^{sym}(\mathbf{k}) := \sum_{\sigma \in S_r} \mathrm{g}(k_{\sigma(1)}, \dots, k_{\sigma(r)}) \in \widetilde{\mathcal{M}}^{\mathbb{Q}}\,,$$

where S_r denotes the set of all permutations of $\{1, \dots, r\}$.

iv) We have

$$\widetilde{\mathcal{M}}^{\mathbb{Q}} = \Big\langle \mathrm{g}^{sym}(k_1, \dots, k_r) \;\Big|\; r \geq 0,\, k_1 \geq k_2 \geq \dots \geq k_r \geq 2 \text{ even} \Big\rangle_{\mathbb{Q}}\,,$$

where we set $\mathrm{g}^{sym}(\emptyset) = 1$.

Proof. This is Exercise 8. The first statement can be proven with Proposition 1.29 and 1.30 by giving explicit formulas for $q\frac{d}{dq}\mathrm{g}(2), q\frac{d}{dq}\mathrm{g}(4)$ and $q\frac{d}{dq}\mathrm{g}(6)$ as polynomials in $\mathrm{g}(2), \mathrm{g}(4)$ and $\mathrm{g}(6)$. From this one also deduces ii). Statement iii) and iv) can be proven by induction on r and the weight respectively. ☐

2.3.5 Linear maps induced by power series

In this section, we want to illustrate an important tool for quasi-shuffle algebras, which was first established in [H2] and later generalized in [HI, Section 3]. Also, there is a recent work of Yamamoto [Y], which generalizes this construction even more and which gives a nice reinterpretation of some of the results we will mention here. One motivation to study these maps is the following: For a given quasi-shuffle algebra $(k\langle A\rangle, *_\diamond)$, one can always construct an explicit isomorphism (of k-algebras) to $(k\langle A\rangle, ⧢)$. In other words, all quasi-shuffle algebras over the same alphabet are isomorphic.
We will first illustrate this the basic idea on multiple zeta values, which are the image of an algebra homomorphism from $(\mathbb{Q}A_z, *)$ to $\mathbb{R}$. We will ignore convergence issues for now, since everything we are going to do could also be done for the truncated version ζ_M. Recall that stuffle product formulas in small depths are given by

$$\begin{aligned} \zeta(k_1)\zeta(k_2) &= \zeta(k_1,k_2)+\zeta(k_2,k_1)+\zeta(k_1+k_2) \\ \zeta(k_1)\zeta(k_2,k_3) &= \zeta(k_1,k_2,k_3)+\zeta(k_2,k_1,k_3)+\zeta(k_2,k_3,k_1)+\zeta(k_1+k_2,k_3)+\zeta(k_2,k_1+k_3)\,. \end{aligned} \tag{2.15}$$

Now one could ask for a new object $S(k_1,\dots,k_r)\in\mathbb{R}$, which does not satisfy the stuffle product formula, but the index shuffle product formula, i.e. which is an image of an algebra homomorphism from $(\mathbb{Q}A_z, ⧢)$ to $\mathbb{R}$. By this we mean we want to construct something out of the multiple zeta values which satisfies in low depths

$$\begin{aligned} S(k_1)S(k_2) &= S(k_1,k_2)+S(k_2,k_1)\,, \\ S(k_1)S(k_2,k_3) &= S(k_1,k_2,k_3)+S(k_2,k_1,k_3)+S(k_2,k_3,k_1)\,. \end{aligned} \tag{2.16}$$

One can check easily that $S(k)=\zeta(k)$ and

$$\begin{aligned} S(k_1,k_2) &= \zeta(k_1,k_2)+\frac{1}{2}\zeta(k_1+k_2)\,, \\ S(k_1,k_2,k_3) &= \zeta(k_1,k_2,k_3)+\frac{1}{2}\zeta(k_1+k_2,k_3)+\frac{1}{2}\zeta(k_1,k_2+k_3)+\frac{1}{6}\zeta(k_1+k_2+k_3)\,, \end{aligned} \tag{2.17}$$

satisfy the index-shuffle product formula (2.16) as a consequence of the stuffle product formula (2.15). One might guess, that this works in arbitrary depths and that the coefficients are given by $\frac{1}{n!}$, whenever one adds together n indices. Since $\frac{1}{n!}$ is the coefficient of T^n in $\exp(T)$ one might think of the above constructions as some exponential map $\exp : (\mathbb{Q}A_z, ⧢)\to(\mathbb{Q}A_z,*)$, which gives us the algebra homomorphism $S:(\mathbb{Q}A_z, ⧢)\to\mathbb{R}$ by setting $S=\zeta\circ\exp$. In this section we want to make this precise, by associating to some power series $f\in Tk[[T]]$ a linear map $\Psi_f : k\langle A\rangle\to k\langle A\rangle$. In the case $f(T)=\exp(T)-1$ we will get the map in the example above.

Now let $w=a_1a_2\cdots a_n$ be a word of length $\ell(w)=n$ with letters $a_1,\dots,a_n\in A$. Let $I=(i_1,\dots,i_m)$ be a composition of n, i.e. $i_1+\dots+i_m=n$ with $m\geq 1$, $i_1,\dots,i_m\geq 1$. For such an I we define

$$I[w]=(a_1\diamond\cdots\diamond a_{i_1})(a_{i_1+1}\diamond\cdots\diamond a_{i_1+i_2})\dots(a_{i_1+\dots+i_{m-1}}\diamond\cdots\diamond a_n)\,.$$

For example for $w=a_1a_3a_3$ a composition of $n=3$ is given by $I=(1,2)$, and we get $I[w]=a_1(a_2\diamond a_3)$. By $\mathcal{C}(n)$ we denote the set of all compositions of n and usually n will be given by the length $n=\ell(w)$ of some word w.

Definition 2.26. *For a formal power series $f=\sum_{i=1}^\infty c_iT^i\in Tk[[T]]$ we define the k-linear map $\Psi_f : k\langle A\rangle\to k\langle A\rangle$ by $\Psi_f(1)=1$ and*

$$\Psi_f(w)=\sum_{I=(i_1,\dots,i_m)\in\mathcal{C}(\ell(w))} c_{i_1}\cdots c_{i_m} I[w]$$

for a nonempty word w.

For example for words of length 2 and 3 we have $\mathcal{C}(2) = \{(1,1),(2)\}$ and $\mathcal{C}(3) = \{(1,1,1),(2,1),(1,2),(3)\}$ which gives for $a_1, a_2, a_3 \in A$

$$\begin{aligned}\Psi_f(a_1 a_2) &= c_1^2\, a_1 a_2 + c_2\, a_1 \diamond a_2\,,\\ \Psi_f(a_1 a_2 a_3) &= c_1^3\, a_1 a_2 a_3 + c_1 c_2\, \big((a_1 \diamond a_2) a_3 + a_1 (a_2 \diamond a_3)\big) + c_3\, a_1 \diamond a_2 \diamond a_3\,.\end{aligned}$$

Observe the similarity of this to (2.17) when $A = A_z$, $z_i \diamond z_j = z_{i+j}$ and $c_i = \frac{1}{i!}$, i.e. $f(T) = \exp(T) - 1$. In the case $f = T$, we obtain the identity map on $k\langle A\rangle$, i.e. $\Psi_f(w) = w$ for all $w \in k\langle A\rangle$. Now for $f, g \in Tk[[T]]$ denote by $f \circ g \in Tk[[T]]$ the usual composition of formal power series, i.e. the power series given by $(f \circ g)(T) = f(g(T))$.

Theorem 2.27. *For $f, g \in Tk[[T]]$ we have*

$$\Psi_f \Psi_g = \Psi_{f \circ g}\,.$$

Proof. This can be found in [HI, Theorem 3.1] and follows from a straightforward but tedious calculation, which we will omit here. □

One interesting case of the linear maps Ψ_f and Ψ_g is given by $f(T) = \exp(T) - 1$ and $g(T) = \log(1+T)$. In these cases we have $(f \circ g)(T) = (g \circ f)(T) = T$ and therefore Ψ_f and Ψ_g are inverse to each other by Theorem 2.27. As in [HI] we write $\exp := \Psi_f$ and $\log := \Psi_g$, i.e. $\exp, \log \in \mathrm{Hom}(k\langle A\rangle, k\langle A\rangle)$. As illustrated in the introduction of this subsection we have the following result, which was first proven in [H1].

Theorem 2.28. *The map*

$$\exp : (k\langle A\rangle, ⧢) \longrightarrow (k\langle A\rangle, *_\diamond)$$

is an k-algebra isomorphism with inverse

$$\log : (k\langle A\rangle, *_\diamond) \longrightarrow (k\langle A\rangle, ⧢)\,.$$

Proof. This is [H1, Theorem 2.5]. □

Theorem 2.28 will be used in Section 5 in the construction of shuffle regularized multiple Eisenstein series, which were introduced in [BT]. Another application will be the proof of Proposition 2.21, which we will do now. For this, we will first give a more general statement on the linear maps Ψ_f.

Proposition 2.29. *For $f \in Tk[[T]]$ and $z \in kA[[X]]$ we have the following equality in $k\langle A\rangle[[X]]$*

$$\Psi_f\left(\frac{1}{1 - zX}\right) = \frac{1}{1 - f_\diamond(zX)}\,.$$

Here Ψ_f acts on $k\langle A\rangle[[X]]$ component wise.

Proof. Let $f(T) = \sum_{i=1}^\infty c_i T^i$, then the left-hand side is given by

$$\begin{aligned}\Psi_f\left(\frac{1}{1 - zX}\right) &= \Psi_f\left(1 + zX + z^2X^2 + z^3X^3 + \dots\right)\\ &= 1 + \sum_{n\geq 1} \sum_{I=(i_1,\dots,i_m)\in\mathcal{C}(n)} c_{i_1}\cdots c_{i_m} I[z^n] X^n\\ &= 1 + \sum_{n\geq 1}\sum_{i_1=1}^{\infty} c_{i_1} \underbrace{z\diamond\cdots\diamond z}_{i_1} X^{i_1} \sum_{I=(i_2,\dots,i_m)\in\mathcal{C}(n-i_1)} c_{i_2}\cdots c_{i_m} I[z^{n-i_1}] X^{n-i_1}\,,\end{aligned}$$

where the last sum on the right needs to be interpreted as 1 in the case $n = i_1$ and 0 if $i_1 > n$. Also notice that I has been extended linearly to $k\langle A\rangle$ and it acts on $k\langle A\rangle[[X]]$ component wise. Now recall that $f_\diamond(zX) = \sum_{i=1}^\infty c_i \underbrace{z \diamond \cdots \diamond z}_{i} X^i$. With this the above equation gives

$$\Psi_f\left(\frac{1}{1-zX}\right) = 1 + f_\diamond(zX)\Psi_f\left(\frac{1}{1-zX}\right),$$

from which the statement follows. □

We can use this Proposition together with Theorem 2.28 to prove Proposition 2.21.

Proof of Proposition 2.21. First notice that for $f(T) = \exp(T) - 1$ the left-hand side of Proposition 2.29 is given by

$$\Psi_f\left(\frac{1}{1-zX}\right) = \exp\left(\frac{1}{1-zX}\right).$$

On the other hand we have

$$\begin{aligned}\frac{1}{1-zX} &= 1 + zX + z^2X^2 + z^3X^3 + \dots \\ &= 1 + zX + \frac{1}{2!}\left(z \sqcup\!\sqcup z\right)X^2 + \frac{1}{3!}\left(z \sqcup\!\sqcup z \sqcup\!\sqcup z\right)X^3 + \dots = \exp_{\sqcup\!\sqcup}(zX)\,.\end{aligned}$$

By Theorem 2.28 $\exp : (k\langle A\rangle, \sqcup\!\sqcup) \longrightarrow (k\langle A\rangle, *_\diamond)$ is an algebra homomorphism and we get

$$\exp\left(\frac{1}{1-zX}\right) = \exp\left(\exp_{\sqcup\!\sqcup}(zX)\right) = \exp_{*_\diamond}(zX)\,,$$

which gives for any $z \in kA[[X]]$ by Proposition 2.29

$$\exp_{*_\diamond}(zX) = \frac{1}{1-\exp_\diamond(zX)}\,.$$

Since this holds for any $z \in kA[[X]]$, the zX can be replaced by any power series in $XkA[[X]]$, i.e. in particular we can choose $\log_\diamond(1+zX) \in XkA[[X]]$ for any $z \in kA[[X]]$, to get

$$\exp_{*_\diamond}(\log_\diamond(1+zX)) = \frac{1}{1-\exp_\diamond(\log_\diamond(1+zX))} = \frac{1}{1-zX}\,,$$

which is exactly the statement of Propositition 2.21. □

2.3.6 Subalgebras of words with restricted first and last letters.

Now we will present a general statement for quasi-shuffle algebras, which we will use to regularize multiple zeta values in the next section. Since multiple zeta values $\zeta(k_1,\dots,k_r)$ are just defined for indices with $k_1 \geq 2$, the map ζ was just defined on $\mathfrak{H}^0$. The subspace $\mathfrak{H}^0$ is spanned by words starting in x and ending in y, or, when viewed as words in A_z, spanned by words not starting in the letter z_1. We want to extend this map to all indices, i.e. to the space $\mathfrak{H}^1$. For example to make sense of ζ for the element z_1z_2 one first notices that

$$z_2 * z_1 = z_2z_1 + z_1z_2 + z_3\,,$$

i.e. $z_1 z_2 = z_2 * z_1 - z_2 z_1 - z_3$ is a polynomial in z_1 (with respect to $*$) with coefficients in $\mathfrak{H}^0$. We will then view z_1 as a variable T and define the stuffle regularized mutliple zeta value as the polynomial $\zeta^*(1,2;T) = \zeta(2)T - \zeta(2,1) - \zeta(3)$, which will give us an algebra homomorphism $\zeta^* : \mathfrak{H}^1_* \to \mathcal{Z}[T]$. This we will do in the next section after proving a general statement for quasi-shuffle algebras in the following, which assures that a polynomial representation as above is possible in certain cases.

For subsets $S, E \subset A$ we define the following subspace of our quasi-shuffle algebra $Q = k\langle A\rangle$

$$\begin{aligned} Q_S^E &= \mathbb{Q} + \langle a_1 a_2 \dots a_n \mid a_1 \in S, a_2, \dots, a_{n-1} \in A, a_n \in E\,, n \geq 1\rangle_{\mathbb{Q}} \\ &= \mathbb{Q} + SQE\,, \end{aligned}$$

i.e. this is the subspace of $k\langle A\rangle$ of words starting with letters in S and ending with letters in in E. In particular we have $Q_A^A = Q$ and we omit writing S or E if they equal A, i.e. $Q_S = Q_S^A$, $Q^E = Q_A^E$.

Proposition 2.30. *If $(kS, \diamond)$ and $(kE, \diamond)$ are subalgebras of $(kA, \diamond)$, then $(Q_S^E, *_\diamond)$ is a subalgebra of $(Q, *_\diamond)$.*

Proof. This is again a direct consequence of the definition of the quasi-shuffle product

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

since the first letters (resp. last letters) of the elements in this product just come from the first letters (resp. last letters) and their $\diamond$ products. ☐

Theorem 2.31. *Assume $(kS, \diamond)$, $(kE, \diamond)$ are subalgebras of $(kA, \diamond)$ and we have an $a \in A$, such that $A \diamond A\backslash\{a\} \subset k\,(A\backslash\{a\})$.*

i) If $a \in E$ we have $Q^E = Q^E_{A\backslash\{a\}}[a]$ and the the map[4]

$$\begin{aligned} \mathrm{pol}_a : Q^E &\longrightarrow Q^E_{A\backslash\{a\}}[T] \\ a &\longmapsto T \end{aligned}$$

is an isomorphism of k-algebras.

ii) If $a \in S$ we have $Q_S = Q_S^{A\backslash\{a\}}[a]$ and the the map

$$\begin{aligned} \mathrm{pol}^a : Q_S &\longrightarrow Q_S^{A\backslash\{a\}}[T] \\ a &\longmapsto T \end{aligned}$$

is an isomorphism of k-algebras.

Proof. For i) we first we want to show that $Q^E = Q^E_{A\backslash\{a\}}[a]$, so we need to show that any word $w \in Q^E$ is a polynomial in a (with respect to the product $*_\diamond$) with coefficients given by linear combination of words not starting in a. We write $w = a^m v$ for $m \geq 0$ and $v = b_1 \cdots b_l \in Q^E_{A\backslash\{a\}}$ and prove the statement by induction on m, where the $m = 0$ case is clear since $w = v \in Q^E_{A\backslash\{a\}}$. By the definition of the quasi-shuffle product we obtain

$$a *_\diamond a^{m-1} v = m\, a^m v + a^{m-1} b_1 (a \sqcup\!\sqcup b_2 \cdots b_l) + \sum_{j=0}^{m-2} a^j (a \diamond a) a^{m-2-j} v + a^{m-1} \sum_{i=1}^{l} b_1 \cdots (a \diamond b_i) \cdots b_l\,.$$

[4]In other words, the polynomial $\sum_{j=0}^m w_j *_\diamond a^{*_\diamond j}$ with $w_j \in Q^E_{A\backslash\{a\}}$ gets send to $\sum_{j=0}^m w_j T^j$.

The last three terms are linear combinations of words starting with a^j with $0 \leq j < m$. Here we used for the last sum the condition $a \diamond b_1 \in kA\backslash\{a\}$. Also all words end with letters in E, since $a, b_l \in E$ and therefore $a \diamond b_l \in kE$. Therefore by the induction hypothesis we get that $w = a^m v$ is also an element in $Q^E_{A\backslash\{a\}}[a]$. To show that the given maps are isomorphism we therefore just need to show that the representation as such a polynomial is unique, i.e. the given maps are injective. But this follows from the fact that there are no linear relations among the elements in $Q^E_{A\backslash\{a\}}$. Since assuming that $0 = \sum_{j=0}^m w_j *_\diamond a^{*_\diamond m}$ with $w_j \in Q^E_{A\backslash\{a\}}$ we immediately get that $w_m = 0$ since it is the only part which gives words starting with a^m. We omit the proof of ii), since the argument for ii) is exactly the same, except that we consider words ending in a^m instead of starting in a^m. □

Theorem 2.31 can be used the prove the following statements, for the spaces $\mathfrak{H}^0$,$\mathfrak{H}^1$,$\mathfrak{H}$ and the products $ш$, $*$ and $*_{\hat\diamond}$. The first two statements are classical results and the last one can be found in [BK1, Theorem 2.14].

Corollary 2.32. *We have*

i) $\mathfrak{H}^1_ш = \mathfrak{H}^0_ш[y]$ *and* $\mathfrak{H}_ш = \mathfrak{H}^1_ш[x] = \mathfrak{H}^0_ш[x, y]$.

ii) $\mathfrak{H}^1_* = \mathfrak{H}^0_*[z_1]$.

iii) $\mathfrak{H}^1_{\hat{*}} = \mathfrak{H}^0_{\hat{*}}[z_1]$.

Proof. In all cases we have $k = \mathbb{Q}$. For *i)* we choose $A = \{x, y\}$, $S = \{x\}$, $E = \{y\}$ and use the trivial product for $\diamond$. With this we have $\mathfrak{H} = Q$, $\mathfrak{H}^1 = Q^E$ and $\mathfrak{H}^0 = Q^E_S$. The statement then follows from Theorem 2.31 i) and ii). For ii) and iii) we choose $A = A_z$, $a = z_1$ and the usual stuffle product for ii) and the quasi-shuffle product $\hat{*}$ for iii). The latter one was defined by using the following product $\hat\diamond$ on kA_z

$$z_{k_1} \hat\diamond z_{k_2} = z_{k_1+k_2} + \sum_{j=1}^{k_1+k_2-1} \left(\lambda^j_{k_1,k_2} + \lambda^j_{k_2,k_1}\right) z_j$$

where the rational numbers $\lambda^j_{k_1,k_2}$ are given by

$$\lambda^j_{k_1,k_2} = (-1)^{k_2-1} \binom{k_1 + k_2 - 1 - j}{k_1 - j} \frac{B_{k_1+k_2-j}}{(k_1 + k_2 - j)!} .$$

By the definition of the $\lambda^j_{k_1,k_2}$ one checks that $\lambda^1_{k_1,k_2} + \lambda^1_{k_2,k_1} = 0$ whenever $k_1 + k_2 \geq 2$ (By using the equation (2.10) in the proof of Proposition 2.20). This shows that $z_1 \hat\diamond A\backslash\{z_1\} \subset \mathbb{Q}A\backslash\{z_1\}$ and we can apply Theorem 2.31. □

Example 2.33. *As an example of Corollary 2.4.3 i), ii) and iii) we give the following expressions of* $z_1z_1z_2$ *as a polynomial in* $z_1 = y$ *having coefficients in* $\mathfrak{H}^0$ *with respect to the products* $ш$, $*$ *and* $\hat{*}$

$$\begin{aligned}
z_1z_1z_2 &= \frac{1}{2} z_2 ш z_1^{ш2} - 2z_2z_1 ш z_1 + 3z_2z_1z_1 \,, \\
z_1z_1z_2 &= \frac{1}{2} z_2 * z_1^{*2} - (z_2z_1 + z_3) * z_1 + \left(z_2z_1z_1 + z_3z_1 + \frac{1}{2} z_4\right) , \\
z_1z_1z_2 &= \frac{1}{2} z_2 \hat{*} z_1^{\hat{*}2} - (z_2z_1 + z_3 - z_2) \hat{*} z_1 + \left(z_2z_1z_1 + z_3z_1 + \frac{1}{2} z_4 - z_3 - \frac{3}{2} z_2z_1 + \frac{5}{12} z_2\right) .
\end{aligned}$$

Notice that the product $\sqcup\!\sqcup$ here is with respect to the alphabet $A = \{x, y\}$ and not A_z! So for the first statement one should rewrite $z_1z_1z_2 = yyxy$, $z_2z_1 = xyy$, etc. If you want to create more examples and play around with $\sqcup\!\sqcup$, $*$ and $\hat{*}$ you can use the following online tool: `https://www.henrikbachmann.com/shuffle.html`, where these three products are implemented on the space A_z. There one could check the above examples by entering ($sh = \sqcup\!\sqcup$, $st = *$, $gst = \hat{*}$)

```
1/2*[1] sh [1] sh [2] -2*[1] sh [2,1]+ 3*[2,1,1]
1/2*[1] st [1] st [2] -[1] st ([2,1]+[3]) + [2,1,1] + [3,1] + 1/2*[4]
1/2*[1]gst[1]gst[2]-[1]gst([2,1]+[3]-[2])+[2,1,1]+[3,1]+1/2*[4]-[3]-3/2*[2,1]+5/12*[2]
```

which all give the output $(1, 1, 2)$.

2.4 Regularizations

As mentioned already at the beginning of the last section we now want to make sense of multiple zeta values for non-admissible indices by using the previous results on quasi-shuffle algebras.

2.4.1 Stuffle and shuffle regularized multiple zeta values

As a consequence of Theorem 2.31 (Corollary 2.4.3) we have for $\bullet \in \{\sqcup\!\sqcup, *\}$ isomorphism of $\mathbb{Q}$-algebras

$$\mathrm{reg}_\bullet^T : \mathfrak{H}_\bullet^1 \to \mathfrak{H}_\bullet^0[T]\,,$$

which send an element $w = \sum_{j=0}^m w_j \bullet z_1^{\bullet m}$ with $w_j \in \mathfrak{H}^0$ to $\mathrm{reg}_\bullet^T(w) = \sum_{j=0}^m w_j T^m$. This enables us to extend the algebra homomorphism $\zeta : \mathfrak{H}_\bullet^0 \to \mathcal{Z}$ to an algebra homomorphism $\zeta^\bullet : \mathfrak{H}_\bullet^1 \to \mathcal{Z}[T]$ by extending ζ to $\mathfrak{H}_\bullet^0[T]$ and setting $\zeta^\bullet = \zeta \circ \mathrm{reg}_\bullet^T$, i.e. we have the following commutative diagram of $\mathbb{Q}$-algebra homomorphism

$$\begin{tikzcd}
\mathfrak{H}_\bullet^1 \arrow[r, "\mathrm{reg}_\bullet^T"] \arrow[dr, "\zeta^\bullet"'] & \mathfrak{H}_\bullet^0[T] \arrow[d, "\zeta"] \\
 & \mathcal{Z}[T]
\end{tikzcd}$$

Definition 2.34. *Let $\mathbf{k} = (k_1, \ldots, k_r) \in \mathbb{Z}_{\geq 1}$ be any index.*

i) We define the **shuffle regularized multiple zeta value**

$$\zeta^{\sqcup\!\sqcup}(\mathbf{k}; T) = \zeta^{\sqcup\!\sqcup}(k_1, \ldots, k_r; T) := \zeta^{\sqcup\!\sqcup}(z_{\mathbf{k}}) \in \mathcal{Z}[T]$$

In the case $T = 0$ we just write $\zeta^{\sqcup\!\sqcup}(\mathbf{k}) = \zeta^{\sqcup\!\sqcup}(\mathbf{k}; 0)$.[5]

ii) We define the **stuffle regularized multiple zeta value**

$$\zeta^*(\mathbf{k}; T) = \zeta^*(k_1, \ldots, k_r; T) := \zeta^*(z_{\mathbf{k}}) \in \mathcal{Z}[T]$$

In the case $T = 0$ we just write $\zeta^*(\mathbf{k}) = \zeta^*(\mathbf{k}; 0)$.

From Example 2.33 we obtain

$$\zeta^{\sqcup\!\sqcup}(1, 1, 2; T) = \frac{1}{2}\zeta(2)T^2 - 2\zeta(2, 1)T + 3\zeta(2, 1, 1)\,,$$
$$\zeta^*(1, 1, 2; T) = \frac{1}{2}\zeta(2)T^2 - (\zeta(2, 1) + \zeta(3))T + \zeta(2, 1, 1) + \zeta(3, 1) + \frac{1}{2}\zeta(4)\,.$$

[5]In the literature often "shuffle/shuffle regularized multiple zeta value" refers to the $T = 0$ case.

Even though the coefficients of T^2 and T are the same (because we know $\zeta(2,1)=\zeta(3)$), the constant terms differ. In general $\zeta^{\sqcup\!\sqcup}(\mathbf{k};T)$ and $\zeta^{\sqcup\!\sqcup}(\mathbf{k};T)$ are different if $\mathbf{k}$ is non-admissible. But we will see in the next section that there is an explicit relationship between these polynomials. Further, we will see in Section 3, that we have for $w\in\mathfrak{H}^0, v\in\mathfrak{H}^1$and $\bullet\in\{\sqcup\!\sqcup,*\}$ the extended double shuffle relations

$$\zeta^{\bullet}(w \sqcup\!\sqcup v - w * v) = 0\,.$$

Since $\zeta^{\sqcup\!\sqcup}$ and ζ^* differ on $\mathfrak{H}^1$ this is not obvious at all. For example, we have (Exercise 9)

$$\zeta^{\bullet}(z_2 \sqcup\!\sqcup z_1z_1 - z_2 * z_1z_1) = 0\,,$$

which implies linear relations among multiple zeta values in weight four.

2.4.2 Comparison of $\zeta^{\sqcup\!\sqcup}$ and ζ^*

As we saw before, the two regularization $\zeta^{\sqcup\!\sqcup}(\mathbf{k};T)$ and $\zeta^*(\mathbf{k};T)$ differ as elements in $\mathbb{R}[T]$. In this section, we will present the exact relationship between these two regularizations as it was done in [IKZ]. For this first consider the following series

$$\begin{aligned} A(u) &= \exp\left(\sum_{n=2}^{\infty}\frac{(-1)^n}{n}\zeta(n)u^n\right)\\ &= 1+\frac{\zeta(2)}{2}u^2-\frac{\zeta(3)}{3}u^3+\left(\frac{\zeta(4)}{4}+\frac{\zeta(2)^2}{8}\right)u^4-\left(\frac{\zeta(5)}{5}+\frac{\zeta(2)\zeta(3)}{6}\right)u^5+\dots\\ &=: \sum_{k\geq 0}\gamma_k\,u^k\,. \end{aligned}$$

Here the $\gamma_k\in\mathbb{Q}[\zeta(j)\mid j\geq 2]$ are polynomials of single zeta values which, considered as multiple zeta values, have homogeneous weight k. Using this we define the $\mathbb{R}$-linear map $\rho:\mathbb{R}[T]\to\mathbb{R}[T]$ by

$$\rho(e^{Tu}) := A(u)e^{Tu}\,. \tag{2.18}$$

Notice that this defines the linear map ρ uniquely by comparing the coefficients of u^m on both sides. Since ρ is linear, we get

$$\begin{aligned} \rho(e^{Tu}) &= \rho(1)+\rho(T)u+\frac{1}{2}\rho(T^2)u^2+\frac{1}{3!}\rho(T^3)u^3+\dots\\ &:= \left(1+\gamma_1u+\gamma_2u^2+\dots\right)\left(1+\frac{1}{2}u^2+\frac{1}{3!}u^3+\dots\right) = A(u)e^{Tu}\,, \end{aligned}$$

and therefore we obtain for $m\geq 0$ the explicit formula

$$\rho\left(T^m\right) = m!\sum_{k=0}^{m}\gamma_k\frac{T^{m-k}}{(m-k)!}\,.$$

Also notice that ρ is bijective. For the first values of m we get

$$
\begin{aligned}
\rho(1) &= 1\,,\\
\rho(T) &= T\,,\\
\rho(T^2) &= T^2 + \zeta(2)\,,\\
\rho(T^3) &= T^3 + 3\zeta(2)T - 2\zeta(3)\,,\\
\rho(T^4) &= T^4 + 6\zeta(2)T^2 - 8\zeta(3)T + 6\zeta(4) + 3\zeta(2)^2\,,\\
\rho(T^5) &= T^5 + 10\zeta(2)T^3 - 20\zeta(3)T^2 + \left(30\zeta(4) + 15\zeta(2)^2\right)T - 24\zeta(5) - 20\zeta(2)\zeta(3)\,.
\end{aligned}
$$

The stuffle regularized multiple zeta values are elements in $\mathbb{R}[T]$ and for example we saw that

$$\zeta^*(1,1,2;T) = \frac{1}{2}\zeta(2)T^2 - (\zeta(2,1)+\zeta(3))T + \zeta(2,1,1) + \zeta(3,1) + \frac{1}{2}\zeta(4)\,.$$

Applying the linear map ρ to this, we see that we just get an additional contribution of $\frac{1}{2}\zeta(2)^2$, i.e.

$$\rho\left(\zeta^*(1,1,2;T)\right) = \frac{1}{2}\zeta(2)T^2 - (\zeta(2,1)+\zeta(3))T + \zeta(2,1,1) + \zeta(3,1) + \frac{1}{2}\zeta(4) + \frac{1}{2}\zeta(2)^2\,.$$

Using the known relations $\zeta(3) = \zeta(2,1)$ and $\zeta(4) = \zeta(2,1,1)$ (duality), $\zeta(3,1) = \frac{1}{4}\zeta(4)$ (finite double shuffle) and $\zeta(2)^2 = \frac{5}{2}\zeta(4)$ (Euler), we get

$$
\begin{aligned}
\rho\left(\zeta^*(1,1,2;T)\right) &= \frac{1}{2}\zeta(2)T^2 - 2\zeta(2,1)T + 3\zeta(2,1,1)\\
&= \zeta^{\sqcup\!\sqcup}(1,1,2;T)\,,
\end{aligned}
$$

i.e. the ρ sends the stuffle regularized multiple zeta value to the shuffle regularized multiple zeta value. In general the map ρ has this property and we have the following

Theorem 2.35. *For all $\mathbf{k} \in \mathbb{Z}^r_{\geq 1}$ we have*

$$\zeta^{\sqcup\!\sqcup}(\mathbf{k};T) = \rho\left(\zeta^*(\mathbf{k};T)\right)\,.$$

Or equivalently, when viewed as maps from $\mathfrak{H}^1$ to $\mathbb{R}[T]$, we have $\zeta^{\sqcup\!\sqcup} = \rho \circ \zeta^*$.

Proof. This is [IKZ, Theorem 1] and we just give a sketch of the proof here. A really detailed version of this proof can also be found in the book of Zhao [Zh1, Section 3.3.2]. The main idea is to compare the behavior of the truncated multiple zeta values $\zeta_M(\mathbf{k})$ (which satisfy the stuffle product formula for all $\mathbf{k}$) and the multiple polylogarithm $\mathrm{Li}_{\mathbf{k}}(z)$ (which satisfy the shuffle product formula for all $\mathbf{k}$) as $M \to \infty$ and $z \to 1$. We have the classical formula

$$\zeta_M(1) = 1 + \frac{1}{2} + \cdots + \frac{1}{M-1} = \log(M) + \gamma + \mathrm{O}\left(\frac{1}{M}\right),$$

as $M \to \infty$, where $\gamma = 0.57721\ldots$ denotes the Euler–Mascheroni constant. As a consequence of the stuffle product formula one can show by induction that for some J we have (see [Zh1, Lemma 3.3.19])

$$\zeta_M(\mathbf{k}) = \zeta^*(\mathbf{k};\log(M)+\gamma) + \mathrm{O}(M^{-1}\log^J(M)) \qquad (\text{as } M \to \infty)\,. \tag{2.19}$$

Similalry by $\mathrm{Li}_1(z) = \log\left(\frac{1}{1-z}\right)$ and using the shuffle product formula for Li one can show, together with the fact that for admissible $\mathbf{k}$ we have $\mathrm{Li}_{\mathbf{k}}(1) - \mathrm{Li}_{\mathbf{k}}(z) = \mathrm{O}(1-z)$, that (see [Zh1, Lemma 3.3.20])

$$\mathrm{Li}_{\mathbf{k}}(z) = \zeta^{ш}\left(\mathbf{k}, \log\left(\frac{1}{1-z}\right)\right) + \mathrm{O}\left((1-z)\log^J\left(\frac{1}{1-z}\right)\right) \qquad (\text{as } z \to 1)\,.$$

The connection of the multiple polylogarithm to the truncated multiple zeta values is, that these basically give the taylor coefficients of $\mathrm{Li}_{\mathbf{k}}$:

$$\begin{aligned}\mathrm{Li}_{\mathbf{k}}(z) = \mathrm{Li}_{k_1,\dots,k_r}(z) &= \sum_{m_1 > \dots > m_r > 0} \frac{z^{m_1}}{m_1^{k_1} \cdots m_r^{k_r}} = \sum_{m=1}^{\infty} \left(\sum_{m > m_2 > \dots > m_r > 0} \frac{1}{m^{k_1} m_2^{k_2} \cdots m_r^{k_r}} \right) z^m \\ &= \sum_{m=1}^{\infty} \left(\zeta_{m+1}(\mathbf{k}) - \zeta_m(\mathbf{k})\right) z^m = (1-z) \sum_{m=1}^{\infty} \zeta_m(\mathbf{k}) z^{m-1}\,.\end{aligned}$$

The statement then follows from the following general fact, that for any polynomial $P(T) \in \mathbb{R}[T]$ and $Q(T) = \rho(P(T))$ one has (see [IKZ, Lemma 1] or [Zh1, Lemma 3.3.17])

$$(1-z)\sum_{m=1} P\left(\log(m) + \gamma\right) z^{m-1} = Q\left(\log\left(\frac{1}{1-z}\right)\right) + \mathrm{O}\left((1-z)\log^J\left(\frac{1}{1-z}\right)\right) \qquad (\text{as } z \to 1)$$

for $J = \deg(P) - 1$ and for $l \geq 0$

$$\sum_{m=1}^{\infty} \frac{\log^l(m)}{m} z^{m-1} = \mathrm{O}\left(\log^{l+1}\left(\frac{1}{1-z}\right)\right) \qquad (\text{as } z \to 1)\,.$$

Choosing $P(T) = \zeta^*(\mathbf{k};T)$ and combining all the equations above gives $Q(T) = \zeta^{ш}(\mathbf{k};T)$ and therefore $\zeta^{ш}(\mathbf{k};T) = \rho(\zeta^*(\mathbf{k};T))$. □

2.4.3 The q-series g for admissible indices

We defined the q-series $g(\mathbf{k})$ for any index $\mathbf{k} = (k_1, \dots, k_r)$ by

$$\begin{aligned}\mathrm{g}(\mathbf{k}) = \mathrm{g}(k_1,\dots,k_r) &= \sum_{m_1 > \dots > m_r > 0} \frac{P_{k_1}(q^{m_1})}{(1-q^{m_1})^{k_1}} \cdots \frac{P_{k_r}(q^{m_r})}{(1-q^{m_r})^{k_r}} \\ &= \sum_{\substack{m_1 > \dots > m_r > 0 \\ d_1,\dots,d_r > 0}} \frac{d_1^{k_1-1}}{(k_1-1)!} \cdots \frac{d_r^{k_r-1}}{(k_r-1)!}\, q^{m_1 d_1 + \dots + m_r d_r}\,.\end{aligned}$$

Only for admissible indices we could consider the limit $q \to 1$ to obtain multiple zeta values, i.e for an admissible index $\mathbf{k}$ we have

$$\lim_{q \to 1} (1-q)^{\mathrm{wt}(\mathbf{k})}\, \mathrm{g}(\mathbf{k}) = \zeta(\mathbf{k})\,. \tag{2.20}$$

Motivated by this, we define for $k \geq 0$ the following spaces

$$\begin{aligned}\mathcal{G}^0 &= \left\langle\, \mathrm{g}(\mathbf{k}) \mid \mathbf{k} \text{ admissible index} \right\rangle_{\mathbb{Q}}\,, \\ \mathcal{G}^0_{\leq k} &= \left\langle\, \mathrm{g}(\mathbf{k}) \mid \mathbf{k} \text{ admissible index}, \mathrm{wt}(\mathbf{k}) \leq k \right\rangle_{\mathbb{Q}}\,.\end{aligned}$$

With this we define for $k \geq 0$ the linear map Z_k

$$\mathrm{Z}_k : \mathcal{G}^0_{\leq k} \longrightarrow \mathcal{Z}_k \tag{2.21}$$
$$f \longmapsto \lim_{q\to 1}(1-q)^k f\,. \tag{2.22}$$

By (2.20) this map is surjective. We now want to extend the map Z_k to all $\mathcal{G}$, i.e. to the space

$$\mathcal{G}_{\leq k} = \big\langle\, \mathrm{g}(\mathbf{k}) \mid \mathbf{k} \text{ index}, \mathrm{wt}(\mathbf{k}) \leq k \big\rangle_{\mathbb{Q}}\,.$$

Considered as a $\mathbb{Q}$-linear map $\mathrm{g} : \mathfrak{H}^1 \to \mathcal{G}$, where $\mathrm{g}(z_{\mathbf{k}}) = \mathrm{g}(\mathbf{k})$, we saw that this gives an algebra homormorphism from $\mathfrak{H}^1_{\hat{*}}$ to $\mathcal{G}$ and the above space is given by $\mathcal{G}^0 = \mathrm{g}(\mathfrak{H}^0)$. By Corollary 2.4.3 we know that $\mathfrak{H}^1_{\hat{*}} = \mathfrak{H}^0_{\hat{*}}[z_1]$, which gives the following.

Proposition 2.36. *i) We have* $\mathcal{G} = \mathcal{G}^0[\mathrm{g}(1)]$.

ii) $\mathrm{g}(1)$ *is algebraically independent over* $\mathcal{G}^0$.

Proof. Statement i) is a direct consequence of Corollary 2.4.3. For ii) the argument is that $\mathrm{g}(1) = \sum_{m,d\geq 1} q^{dm} \asymp \frac{-\log(1-q)}{1-q}$ as $q \to 1$ and $\mathrm{g}(\mathbf{k}) \asymp \frac{1}{(1-q)^{\mathrm{wt}(\mathbf{k})}}$ for admissible $\mathbf{k}$. Here $f(q) \asymp g(q)$ as $q \to 1$ means that there exist constants $A, B \in \mathbb{R}_{>0}$, such that $A \leq |\frac{f(q)}{g(q)}| \leq B$ as $q \to 1$. Both statements can also be found in [BK1, Theorem 2.14] (see also [P, Lemma 2]). □

Using Proposition 2.36 we can extend for $k \geq 0$ the map Z_k to $\mathcal{G}_{\leq k}$. Since any $f \in \mathcal{G}_{\leq k}$ can be written uniquely as $f = \sum_{j=0}^{k} f_j\, \mathrm{g}(1)^{k-j}$, with $f_j \in \mathcal{G}^0_{\leq j}$. With this we define

$$\mathrm{Z}^T_k : \mathcal{G}_{\leq k} \longrightarrow \mathcal{Z}[T]$$
$$\sum_{j=0}^{k} f_j\ \mathrm{g}(1)^{k-j} \longmapsto \sum_{j=0}^{k} \mathrm{Z}_j(f_j)\, T^{k-j}$$

where $\mathrm{Z}_j(f_j)$ for $f_j \in \mathcal{G}^0_{\leq j}$ is defined by (2.21).

Proposition 2.37. *For any index* $\mathbf{k}$ *we have*

$$\mathrm{Z}^T_{\mathrm{wt}\,(\mathbf{k})}\,(\mathrm{g}(\mathbf{k})) = \zeta^*(\mathbf{k}; T)\,.$$

Proof. Let $w \in \mathfrak{H}^1$. By Corollary we have $\mathfrak{H}^1_* = \mathfrak{H}^0_*[z_1]$ and $\mathfrak{H}^1_{\hat{*}} = \mathfrak{H}^0_{\hat{*}}[z_1]$ and therefore there exist $u_j, v_j \in \mathfrak{H}^0$, such that

$$w = \sum_{j=0}^{m} u_j * z_1^{*j} = \sum_{j=0}^{m} v_j \,\hat{*}\, z_1^{\hat{*}j}\,.$$

Since we have

$$z_{k_1} \hat{\diamond} z_{k_2} = z_{k_1+k_2} + \sum_{j=1}^{k_1+k_2-1} \left(\lambda^j_{k_1,k_2} + \lambda^j_{k_2,k_1}\right) z_j$$

we see, by following the proof of Theorem 2.31, that u_j and v_j just differ by linear combination of words $z_{\mathbf{k}'}$ with indices satisfying $\mathrm{wt}(\mathbf{k}') < j$. Since $\mathcal{G}_{\leq j-1} \subset \ker(\mathrm{Z}_j)$ the statement follows. □

§3 Families of linear relations and their q-relatives

In this section, we want to discuss several families of linear relations among multiple zeta values and also some of their q-analogues. Asking for linear relations among multiple zeta values is equivalent in asking for the kernel of the map $\zeta : \mathfrak{H}^0 \to \mathcal{Z}$.

3.1 Extended double shuffle relations

As an extension of the finite double shuffle relations (Proposition 2.14) we will now present a family of linear relations, which give conjecturally all linear relations among multiple zeta values. We define for $w, u \in \mathfrak{H}^1$ the element

$$\mathrm{ds}(w,u) := w ш u - w * u \in \mathfrak{H}^1 .$$

The statement of Proposition 2.14 then was, that $\mathrm{ds}(w,u) \in \ker \zeta$ if $w, u \in \mathfrak{H}^0$. The extended version states, that one of the words w and u is allowed to be in $\mathfrak{H}^1$. In this case $\mathrm{ds}(w,u)$ is not necessary in $\mathfrak{H}^0$ anymore, but after projecting to $\mathfrak{H}^0$ by the map $\mathrm{reg}_\bullet^T : \mathfrak{H}^1_\bullet \to \mathfrak{H}^0_\bullet[T]$ and then comparing the coefficients of T (or setting $T = 0$, for which we write $\mathrm{reg}_\bullet := \mathrm{reg}_\bullet^0$) one still obtains a relation among multiple zeta values. In other words $\mathrm{ds}(w,u)$ is in the kernel of the regularized multiple zeta value maps.

Theorem 3.1 (Extended double shuffle relations)**.** *For $w \in \mathfrak{H}^1$, $u \in \mathfrak{H}^0$ and $\bullet \in \{ш, *\}$ we have*

$$\zeta^\bullet(w ш u - w * u; T) = 0 ,$$

i.e. in particular $\mathrm{reg}_\bullet (\mathrm{ds}(w,u)) \in \ker \zeta$.

Proof. By Theorem 2.35 we have for all $w \in \mathfrak{H}^1$

$$\zeta^ш(w; T) = \rho\left(\zeta^*(w;T)\right) .$$

Multiplying both sides with $\zeta^ш(u) = \zeta^*(u) = \zeta(u) \in \mathbb{R}$, for $u \in \mathfrak{H}^0$, we get by the $\mathbb{R}$-linearity of ρ

$$\begin{aligned} \zeta^ш(w ш u; T) &= \rho\left(\zeta^*(w * u; T)\right) \\ &= \zeta^ш(w * u; T) . \end{aligned}$$

This gives $\zeta^ш(w ш u - w * u; T) = 0$ and $\zeta^*(w ш u - w * u; T) = 0$ by applying the inverse of ρ. ☐

Conjecture 3.2. *The kernel of $\zeta : \mathfrak{H}^0 \to \mathcal{Z}$ is given by*

$$\begin{aligned} \ker \zeta &= \left\langle \mathrm{reg}_ш \left(w ш u - w * u\right) \mid w \in \mathfrak{H}^1,\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}} \\ &= \left\langle \mathrm{reg}_* \left(w ш u - w * u\right) \mid w \in \mathfrak{H}^1,\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}} , \end{aligned}$$

i.e. the extended double shuffle relations give all $\mathbb{Q}$-linear relations among multiple zeta values.

Since it is expected that the extended double shuffle relations give all relations among multiple zeta values, one could obtain upper bounds for the dimension of $\mathcal{Z}_k$, i.e., an alternative proof of Theorem 1.15, by counting these relations. This is still an open problem.

Open problem 3.3. *Count the number of linearly independent extended double shuffle relations. Define for $k \geq 0$ and $\bullet \in \{ш, *\}$ the spaces*

$$\mathsf{eds}_k^\bullet = \left\langle \operatorname{reg}^\bullet (w ш u - w * u) \mid w \in \mathfrak{H}^1,\, u \in \mathfrak{H}^0, \operatorname{wt}(w) + \operatorname{wt}(u) = k \right\rangle_{\mathbb{Q}}.$$

Show that for all $k \geq 2$ and any $\bullet \in \{ш, *\}$ we have

$$\dim_{\mathbb{Q}} \mathsf{eds}_k^\bullet = 2^{k-2} - d_k\,. \tag{3.1}$$

Here the d_k are the conjectured dimensions (Conjecture 1.13) of $\mathcal{Z}_k$, defined by

$$\sum_{k \geq 0} d_k X^k = \frac{1}{1 - X^2 - X^3}\,,$$

and 2^{k-2} is the number of admissible indices of weight k.

So far the equation (3.1) has been checked up to $k = 21$ (T. Machide, T. Sonobe, 2020+) by extensive computer calculations.
All the relations we obtained so far should be a consequence of the extended double shuffle relations. For the finite double shuffle relations this is obvious, but for the duality relation this is actually also an open problem. Recall that the duality relations (Proposition 2.5) stated that for all $v \in \mathfrak{H}^0$ we have

$$\zeta(\tau(v)) = \zeta(v)\,,$$

where τ was the anti-automorphism defined on $\mathfrak{H}^0$ with $\tau(y) = x$ and $\tau(y) = x$.

Open problem 3.4. *Show that for any $v \in \mathfrak{H}^0$ we have for $\bullet \in \{ш, *\}$*

$$\tau(v) - v \in \left\langle \operatorname{reg}_\bullet (w ш u - w * u) \mid w \in \mathfrak{H}^1,\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}},$$

i.e. the duality relation is a consequence of the extended double shuffle relations.

We now want to discuss a refinement of the extended double shuffle relations. For this, we first consider the following special case.

Proposition 3.5 (Hoffman's relation ([H1]))**.** *For an admissible index $\mathbf{k} = (k_1, \ldots, k_r)$ we have*

$$\sum_{i=1}^{r} \zeta(k_1, \ldots, k_{i-1}, k_i + 1, k_{i+1}, \ldots, k_r) = \sum_{\substack{1 \leq i \leq r \\ k_i \geq 2}} \sum_{j=0}^{k_i - 2} \zeta(k_1, \ldots, k_{i-1}, k_i - j, j + 1, k_{i+1}, \ldots, k_r)\,.$$

Proof. This is a special case of the extended double shuffle relation by choosing $w = z_1 = y$ and $u = z_{\mathbf{k}}$. In particular, we have $\operatorname{ds}(z_1, z_{\mathbf{k}}) \in \mathfrak{H}^0$ (Exercise 10) and therefore no regularization is necessary. Another proof of this relation, using partial fraction decomposition, can be found in [Zu2, Theorem 1]. $\square$

Hoffman's relation is a special case of the extended double shuffle relations, which are not a consequence of the finite double shuffle relations. Surprisingly, it seems that this is the only part of the extended double shuffle relations we need.

Conjecture 3.6 (H. N. Minh, M. Petitot et al. ([MJOP]))**.** *We have*

$$\ker \zeta = \left\langle w ш u - w * u \mid w \in \mathfrak{H}^0 \cup \{z_1\},\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}},$$

i.e. Hoffman's relation and the finite double shuffle relations give all linear relations among multiple zeta values.

But still, this set of relations seems to be too much, and the following gives an even better refinement.

Conjecture 3.7 (M. Kaneko, M.Noro and K.Tsurumaki ([KNT])). *We have*

$$\ker \zeta = \left\langle w ⧢ u - w * u \mid w \in \{z_1, z_2, z_3, z_2 z_1\},\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}}.$$

The equivalence of these conjectures is not known and in particular we have the the following open problem.

Open problem 3.8. *Show that*

$$\begin{aligned}\left\langle \operatorname{reg}_{⧢} (w ⧢ u - w * u) \mid w \in \mathfrak{H}^1,\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}} &= \left\langle \operatorname{reg}_{*} (w ⧢ u - w * u) \mid w \in \mathfrak{H}^1,\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}} \\ &= \left\langle w ⧢ u - w * u \mid w \in \mathfrak{H}^0 \cup \{z_1\},\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}} \\ &= \left\langle w ⧢ u - w * u \mid w \in \{z_1, z_2, z_3, z_2 z_1\},\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}}.\end{aligned}$$

Having an element $w \in \ker \zeta$ and $u \in \mathfrak{H}^0$, then clearly also $w * u, w ⧢ u \in \ker \zeta$. As far as the author knows, it is also still an open problem to show that the space of extended double shuffle relations is closed under the multiplication with elements in $\mathfrak{H}^0$.

Open problem 3.9. *Show that for $\bullet_1, \bullet_2 \in \{⧢, *\}$ we have*

$$\mathfrak{H}^0 \bullet_1 \left\langle \operatorname{reg}_{\bullet_2} (w ⧢ u - w * u) \mid w \in \mathfrak{H}^1,\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}} \subset \left\langle \operatorname{reg}_{\bullet_2} (w ⧢ u - w * u) \mid w \in \mathfrak{H}^1,\, u \in \mathfrak{H}^0 \right\rangle_{\mathbb{Q}}.$$

3.2 Seki-Yamamoto's connected sums and Ohno's relation

In this section, we want to present an alternative proof of the duality relation (Proposition 2.5), which was given by Seki and Yamamoto in [SY][6]. In this nice work, they introduce the notion of connected sums, which recently also found their ways into various other proofs of families of relations among multiple zeta values and some their variants, such as finite multiple zeta values. In [S] you can find an overview of different applications of connected sums. We will use this setup to present a proof of Ohno's relation for q-analogues of multiple zeta values as it was given in [SY].

3.2.1 Connected sums and the duality relation for multiple zeta values

We start by reformulating the duality relations on the level of indices. Recall that $\tau : \mathfrak{H}^0 \to \mathfrak{H}^0$ was defined as the anti-automorphism (with respect to the usual multiplicaton in $\mathbb{Q}\langle x, y\rangle$) satisfying $\tau(x) = y$ and $\tau(y) = x$. Now let $\mathbf{k} = (k_1, \dots, k_r)$ be an admissible index, i.e. $k_1 \geq 2$ and $z_{\mathbf{k}} \in \mathfrak{H}^0$. Then there exist numbers $a_1, b_1, \dots, a_s, b_s \geq 1$, such that

$$\mathbf{k} = (a_1 + 1, \{1\}^{b_1 - 1}, a_2 + 1, \{1\}^{b_2 - 1}, \dots, a_s + 1, \{1\}^{b_s - 1}).$$

With these numbers we define the admissible index $\mathbf{k}^\dagger$ by

$$\mathbf{k}^\dagger := (b_s + 1, \{1\}^{a_s - 1}, b_{s-1} + 1, \{1\}^{a_{s-1} - 1}, \dots, b_1 + 1, \{1\}^{a_1 - 1}).$$

One can then see by induction on s, that we have (Exercise 11)

$$z_{\mathbf{k}^\dagger} = \tau(z_{\mathbf{k}}), \tag{3.2}$$

[6] In the work [SY] the order of summation in the definition of multiple zeta values is reversed. Therefore one needs to be careful when comparing the results here and the ones in their work.

i.e. the duality relation of multiple zeta values can be stated as $\zeta(\mathbf{k}) = \zeta(\mathbf{k}^\dagger)$ for all admissible $\mathbf{k}$. Now we will introduce the connected sum for multiple zeta values. The name comes from the fact that these sums look like the product of two multiple zeta values, which get connected at someplace by a connector.

Definition 3.10. *Let $\mathbf{k} = (k_1, \dots, k_r)$, $\mathbf{l} = (l_1, \dots, l_s)$ be two non-empty indices. Then we define the* **connected sum** $Z(\mathbf{k}; \mathbf{l})$ *by*

$$Z(\mathbf{k}; \mathbf{l}) = Z(k_1, \dots, k_r; l_1, \dots, l_s) = \sum_{\substack{m_1 > m_2 > \dots > m_r > 0 \\ n_1 > n_2 > \dots > n_s > 0}} \frac{m_1!\, n_1!}{(m_1 + n_1)!} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}} \frac{1}{n_1^{l_1} \cdots n_s^{l_s}} \tag{3.3}$$

and set $Z(\mathbf{k}; \emptyset) = Z(\emptyset; \mathbf{k}) = \zeta(\mathbf{k})$ for admissible $\mathbf{k}$.

One can check that the sum (3.3) converges for all non-empty indices $\mathbf{k}$ and $\mathbf{l}$. Also notice that (3.3) is essentially the product $\zeta(\mathbf{k})\zeta(\mathbf{l})$, which gets connected by the **connector** $c(m_1, n_1) = \frac{m_1!\, n_1!}{(m_1+n_1)!}$ at the beginning. The relationship to the duality relations comes from the fact that one can show that $Z(\mathbf{k}; \emptyset) = \dots = Z(\emptyset; \mathbf{k}^\dagger)$, by using the following transport relations.

Proposition 3.11 (Transport relations)**.** *Let $(k_1, \dots, k_r)$ and $(l_1, \dots, l_s)$ be two indices.*
If $s > 0$ then we have

$$Z(1, k_1, \dots, k_r; l_1, \dots, l_s) = Z(k_1, \dots, k_r; l_1 + 1, l_2, \dots, l_s)$$

and if $r > 0$, then we have

$$Z(k_1 + 1, k_2, \dots, k_r; l_1, \dots, l_s) = Z(k_1, \dots, k_r; 1, l_1, l_2, \dots, l_s)\,.$$

Proof. To prove the first equality we use for $m \geq 0$ the telescoping sum

$$\sum_{a=m+1}^{\infty} \frac{1}{a} \frac{a!\, n!}{(a+n)!} = \frac{1}{n} \sum_{a=m+1}^{\infty} \left(\frac{(a-1)!n!}{(a-1+n)!} - \frac{a!n!}{(a+n)!} \right) = \frac{1}{n} \frac{m!n!}{(m+n)!}\,, \tag{3.4}$$

from which we obtain

$$\begin{aligned} Z(1, k_1, \dots, k_r; l_1, \dots, l_s) &= \sum_{\substack{a > m_1 > m_2 > \dots > m_r > 0 \\ n_1 > n_2 > \dots > n_s > 0}} \frac{1}{a} \frac{a!\, n_1!}{(a + n_1)!} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}} \frac{1}{n_1^{l_1} \cdots n_s^{l_s}} \\ &= \sum_{\substack{m_1 > m_2 > \dots > m_r > 0 \\ n_1 > n_2 > \dots > n_s > 0}} \frac{1}{n_1} \frac{m_1!\, n_1!}{(m_1 + n_1)!} \frac{1}{m_1^{k_1} \cdots m_r^{k_r}} \frac{1}{n_1^{l_1} \cdots n_s^{l_s}} \\ &= Z(k_1, \dots, k_r; l_1 + 1, l_2, \dots, l_s)\,. \end{aligned}$$

Also notice that we obtain $Z(1; l_1, \dots, l_s) = Z(\emptyset; l_1 + 1, l_2, \dots, l_s) = \zeta(l_1 + 1, l_2, \dots, l_s)$ here in the case $r = 0$ by using the $m = 0$ case of (3.4). The second statement follows from the symmetry $Z(\mathbf{k}; \mathbf{l}) = Z(\mathbf{l}; \mathbf{k})$. $\square$

Using these transport relations, we can therefore always transport one index from the left to the right and vice-verse. For example, we have

$$\zeta(3) = Z(3; \emptyset) = Z(2; 1) = Z(1; 1, 1) = Z(\emptyset; 2, 1) = \zeta(2, 1)\,.$$

In general the duality relations follows from this, since if we start with an admissible index $\mathbf{k} = (a_1+1, \{1\}^{b_1-1}, a_2+1, \{1\}^{b_2-1}, \dots, a_s+1, \{1\}^{b_s-1})$, we can use a_1-times the second transport relations and b_1-times the first, then a_2-times the second and b_2-times the first, etc., to get

$$\begin{aligned}\zeta(\mathbf{k}) &= Z(a_1+1, \{1\}^{b_1-1}, a_2+1, \{1\}^{b_2-1}, \dots, a_s+1, \{1\}^{b_s-1}; \emptyset) = \dots \\ &= Z(\{1\}^{b_1-1}, a_2+1, \{1\}^{b_2-1}, \dots, a_s+1, \{1\}^{b_s-1}; 2, \{1\}^{a_1-1}) = \dots \\ &= Z(a_2+1, \{1\}^{b_2-1}, \dots, a_s+1, \{1\}^{b_s-1}; b_1+1, \{1\}^{a_1-1}) = \dots \\ &= \dots \\ &= Z(\emptyset; b_s+1, \{1\}^{a_s-1}, b_{s-1}+1, \{1\}^{a_{s-1}-1}, \dots, b_1+1, \{1\}^{a_1-1}) = Z(\emptyset; \mathbf{k}^\dagger) = \zeta(\mathbf{k}^\dagger)\,.\end{aligned} \tag{3.5}$$

3.2.2 The sum formula and Ohno's relation

We will now present a family of linear relations, which are known as Ohno's relation. These types of relations generalize the duality relation and the so-called sum formula, given by the following.

Theorem 3.12 (Sum formula (Granville [G], Zagier))**.** *For all $k \geq 2$ and $1 \leq r < k$ we have*

$$\sum_{\substack{k_1+\dots+k_r=k \\ k_1\geq 2,\, k_2,\dots,k_r \geq 1}} \zeta(k_1, \dots, k_r) = \zeta(k)\,. \tag{3.6}$$

The sum formula therefore states that the sum over all multiple zeta values of weight k in any fixed depths always gives the Riemann zeta value $\zeta(k)$. Notice again, that our first relation $\zeta(2,1) = \zeta(3)$ is also the first (non-trivial) example of the sum-formula. There a various generalization of the sum formula, which for example, also include weights and therefore are called weighted sum formulas.

To state Ohno's relation we first define for an admissible index $\mathbf{k} = (k_1, \dots, k_r)$ the **Ohno sum** by

$$\mathcal{O}^X(\mathbf{k}) = \sum_{c \geq 0} O(\mathbf{k}; c) X^c \in \mathcal{Z}[[X]]\,,$$

where we write for $c \geq 0$

$$O(\mathbf{k}; c) = \sum_{\substack{c_1+\dots+c_r=c \\ c_1,\dots,c_r \geq 0}} \zeta(k_1+c_1, \dots, k_r+c_r) \in \mathcal{Z}_{\mathrm{wt}(\mathbf{k})+c}\,.$$

Notice that for $\mathbf{k} = (2, \{1\}^{r-1})$ and $c = k-r-1$ we obtain the left-hand side of (3.6)

$$O(2, \{1\}^{r-1}; k-r-1) = \sum_{\substack{k_1+\dots+k_r=k \\ k_1\geq 2,\, k_2,\dots,k_r \geq 1}} \zeta(k_1, \dots, k_r)\,.$$

Ohno's relation now states, that the Ohno sum also satisfies the duality relation.

Theorem 3.13 (Ohno's relation (Ohno [Oh]))**.** *For any admissible index $\mathbf{k}$ we have*

$$\mathcal{O}^X(\mathbf{k}) = \mathcal{O}^X(\mathbf{k}^\dagger)\,.$$

Since $\mathcal{O}^0(\mathbf{k}) = O(\mathbf{k}; 0) = \zeta(\mathbf{k})$ we obtain the duality as a special case by considering the constant term in Ohno's relation. Choosing for $r \geq 1$ the index $\mathbf{k} = (2, \{1\}^{r-1})$ we have $\mathbf{k}^\dagger = (r+1)$, and therefore the sum formula (3.6) follows by considering the coefficient of X^{k-r-1} in $\mathcal{O}^X(2,1,\dots,1) = \mathcal{O}^X(r+1)$. The formulation of the Ohno relation in the original work of Ohno is a bit different and we use here the formulation of [HMOS], where the authors also prove further relations of the Ohno sums besides the duality relation.

Example 3.14. *For* $\mathbf{k} = (2,2,1)$ *we have* $\mathbf{k}^\dagger = (3,2)$ *and*

$$\begin{aligned}\mathcal{O}^X(2,2,1) &= \zeta(2,2,1) + \big(\zeta(3,2,1) + \zeta(2,3,1) + \zeta(2,2,2)\big)X \\ &\qquad + \big(\zeta(4,2,1) + \zeta(2,4,1) + \zeta(2,2,3) + \zeta(3,3,1) + \zeta(3,2,2) + \zeta(2,3,2)\big)X^2 + \dots\,, \\ \mathcal{O}^X(3,2) &= \zeta(3,2) + \big(\zeta(4,2) + \zeta(3,3)\big)X + \big(\zeta(5,2) + \zeta(3,4) + \zeta(4,3)\big)X^2 + \dots\,,\end{aligned}$$

which gives linear relation among multiple zeta values of weight $5+c$ *by comparing the coefficients of* X^c *in* $\mathcal{O}^X(2,2,1) = \mathcal{O}^X(3,2)$.

The number of Ohno's relations is given by the following table (calculated by Tanaka in [Tan2]).

weight k	3	4	5	6	7	8	9	10	11	12
# all conjectured relations	1	3	6	14	29	60	123	249	503	1012
# Ohno's relations	1	2	5	10	23	46	98	199	411	830

We now want to state the q-analogue version of Ohno's relation. Recall that we defined for an admissible index $\mathbf{k} = (k_1, \dots, k_r)$ the Bradley-Zhao q-analogues of multiple zeta values by

$$\zeta_q^{\mathrm{BZ}}(\mathbf{k}) = \zeta_q^{\mathrm{BZ}}(k_1, \dots, k_r) = \sum_{m_1 > \dots > m_r > 0} \frac{q^{(k_1-1)m_1} \dots q^{(k_r-1)m_r}}{[m_1]_q^{k_1} \cdots [m_r]_q^{k_r}}\,, \tag{3.7}$$

where $[m]_q = \frac{1-q^m}{1-q}$ denotes the q-integer. It was first shown by Bradley ([Bra]) that these q-series also satisfy Ohno's relation. Define for an admissible index $\mathbf{k} = (k_1, \dots, k_r)$ the **q-Ohno sum** by

$$\mathcal{O}_q^X(\mathbf{k}) = \sum_{c \geq 0} O_q(\mathbf{k}; c) X^c \in \mathbb{Q}[[q]][[X]]\,,$$

where we write for $c \geq 0$

$$O_q(\mathbf{k}; c) = \sum_{\substack{c_1 + \dots + c_r = c \\ c_1, \dots, c_r \geq 0}} \zeta_q^{\mathrm{BZ}}(k_1 + c_1, \dots, k_r + c_r)\,.$$

The series $\mathcal{O}_q^X(\mathbf{k})$ is a formal power-series in X with coefficients given by formal power series in q. For real $0 < q, X < 1$ one can show that $\mathcal{O}_q^X(\mathbf{k})$ converges and gives a well-defined real number.

Theorem 3.15 (Ohno's relation for q-MZV (Bradley [Bra]))**.** *For any admissible index* $\mathbf{k}$ *we have*

$$\mathcal{O}_q^X(\mathbf{k}) = \mathcal{O}_q^X(\mathbf{k}^\dagger)\,.$$

Notice that Theorem 3.15 implies that the q-analogues ζ_q^{BZ} also satisfy the sum-formula and the duality relation. Also sending $q \to 1$ we obtain Ohno's relation for multiple zeta values.

The goal is now to give a proof of Theorem 3.15 by using Seki-Yamamoto's concept of connected sums.

For this we first rewrite the q-Ohno sum as

$$\begin{aligned}\mathcal{O}_q^X(\mathbf{k}) &= \sum_{c\geq 0} O_q(\mathbf{k};c)X^c = \sum_{c_1,\dots,c_r\geq 0} \zeta_q^{\mathrm{BZ}}(k_1+c_1,\dots,k_r+c_r)X^{c_1+\dots+c_r} \\ &= \sum_{\substack{m_1>\dots>m_r>0\\ c_1,\dots,c_r\geq 0}} \frac{q^{(k_1+c_1-1)m_1}\cdots q^{(k_r+c_r-1)m_r}}{[m_1]_q^{k_1+c_1}\cdots[m_r]_q^{k_r+c_r}} X^{c_1+\dots+c_r} \\ &= \sum_{m_1>\dots>m_r>0} \frac{q^{(k_1-1)m_1}}{([m_1]_q-q^{m_1}X)[m_1]_q^{k_1-1}} \cdots \frac{q^{(k_r-1)m_r}}{([m_r]_q-q^{m_r}X)[m_r]_q^{k_r-1}} \\ &= \sum_{m_1>\dots>m_r>0} s_q^X(k_1,m_1)\cdots s_q^X(k_r,m_r)\,,\end{aligned}$$

where we set

$$s_q^X(k,m) = \frac{q^{(k-1)m}}{([m]_q-q^mX)[m]_q^{k-1}}\,. \tag{3.8}$$

Notice that $s_1^0(k,m)=\frac{1}{m^k}$, i.e. the q-Ohno sum reduces to the multiple zeta value $\mathcal{O}_1^0(\mathbf{k})=\zeta(\mathbf{k})$ in this case. To define the connected sum we need to find the correct connector $c_q^X(m,n)$, which generalizes the connector $c_1^0(m,n)=c(m,n)=\frac{m!\,n!}{(m+n)!}$ we used for multiple zeta values. This was done by Seki and Yamamoto in [SY], by choosing the connector

$$c_q^X(m,n) = \frac{q^{mn}f_q^X(m)f_q^X(n)}{f_q^X(m+n)}\,, \tag{3.9}$$

where $f_q^X(m)=\prod_{j=1}^m([j]_q-q^jX)$, which can be seen as a variant of the factorial, since $f_1^0(m)=m!$.

Definition 3.16. *Let $\mathbf{k}=(k_1,\dots,k_r)$, $\mathbf{l}=(l_1,\dots,l_s)$ be two non-empty indices. Then we define the* **connected q-Ohno sum** $\mathcal{O}_q^X(\mathbf{k};\mathbf{l})$ *by*

$$\mathcal{O}_q^X(\mathbf{k};\mathbf{l}) = \sum_{\substack{m_1>m_2>\dots>m_r>0\\ n_1>n_2>\dots>n_s>0}} c_q^X(m_1,n_1)\prod_{i=1}^r s_q^X(k_i,m_i)\prod_{j=1}^s s_q^X(l_j,n_j) \tag{3.10}$$

and set $\mathcal{O}_q^X(\mathbf{k};\emptyset)=\mathcal{O}_q^X(\emptyset;\mathbf{k})=\mathcal{O}_q^X(\mathbf{k})$ for admissible $\mathbf{k}$. The s_q^X and c_q^X are given by (3.8) *and* (3.9)*.*

Proposition 3.17 (q-Transport relations)**.** *Let $(k_1,\dots,k_r)$ and $(l_1,\dots,l_s)$ be two indices. If $s>0$ then we have*

$$\mathcal{O}_q^X(1,k_1,\dots,k_r;l_1,\dots,l_s) = \mathcal{O}_q^X(k_1,\dots,k_r;l_1+1,l_2,\dots,l_s)$$

and if $r>0$, then we have

$$\mathcal{O}_q^X(k_1+1,k_2,\dots,k_r;l_1,\dots,l_s) = \mathcal{O}_q^X(k_1,\dots,k_r;1,l_1,l_2,\dots,l_s)\,.$$

Proof. This proof is Exercise 11 and it is similar to the proof of Proposition 3.11. □

With the same argument as in (3.5) we see that these transport relations imply Theorem 3.15, i.e. $\mathcal{O}_q^X(\mathbf{k})=\mathcal{O}_q^X(\mathbf{k}^\dagger)$.

Remark 3.18. We will see in Section 5 that Theorem 3.15 also implies a version of Ohno's relation for our q-series $\mathrm{g}(\mathbf{k})$. More precisely, we will introduce a double-indexed version $\mathrm{g}\binom{\mathbf{k}}{\mathbf{l}}$, which span the space $\mathcal{Z}_q$, introduced in Section 1.4.3. We then obtain relations in this space since the coefficients of the modified version $(1-q)^{-\operatorname{wt}(\mathbf{k})}\mathcal{O}_q^{(1-q)^{-1}X}(\mathbf{k})$ are also elements in $\mathcal{Z}_q$.

3.3 The zoo of relations

We already studied various relations of multiple zeta values. But there are many more relations, which we will not be able to cover in this course. Instead, we will provide a small overview of some of them and their relationships. In Figure 1, we give an overview of families of linear and algebraic relations among multiple zeta values and some of their implications. This overview was done together with the help of T. Tanaka, and for a more detailed list of results on multiple zeta values, one should have a look at the list of research papers collected by Hoffman in [H0]. Some of the presented relations already appeared before, and for some of them, we will provide a few explanations. For the remaining ones, we refer to the literature. (☕ I will try to add more details & examples in the future)

In the following, we provide references and some explanations of Figure 1.

(1) **Motivic relations:** See [Br].

(2) **Associator relations:** See [D] and [F].

(3) **Confluence relations:** See [HS].

(4) **Integral-Series identity:** See [KY].

(5) **Extended double shuffle relations:** This is Theorem 3.1.

(6) **Kawashima's relations:** Define the automorphism $\varphi \in \mathrm{Aut}(\mathfrak{H})$ (with respect to the concatenation) on the generators by $\varphi(x) = x + y$ and $\varphi(y) = -y$ and define for words $v, w \in \mathfrak{H}y$ the operator $z_p v \circledast z_q w = z_{p+q}(v * w)$. With this the Kawashima relations can be stated as follows:

Theorem 3.19. *([Kaw, Corollary 5.4]) For all $v, w \in \mathfrak{H}y$ and $m \geq 1$ we have*

$$\sum_{\substack{i+j=m \\ i,j \geq 1}} \zeta(\varphi(v) \circledast y^i)\zeta(\varphi(w) \circledast y^j) = \zeta(\varphi(v * w) \circledast y^m)\,. \tag{3.11}$$

It is expected that Theorem 3.19 gives all $\mathbb{Q}$-linear relations between multiple zeta values after evaluating the product on the left-hand side by the shuffle product formula. Moreover, numerical experiment suggests that the two cases $m = 1, 2$ are enough to obtain all linear relations.

(7) **Duality:** This is Proposition 2.5.

(8) **Euler's relations:** This is Proposition 1.1.

(9) **Finite double shuffle relations:** This is Proposition 2.14.

(10) **Shuffle product:** This is Corollary 2.10.

(11) **Stuffle product:** This is Corollary 2.13.

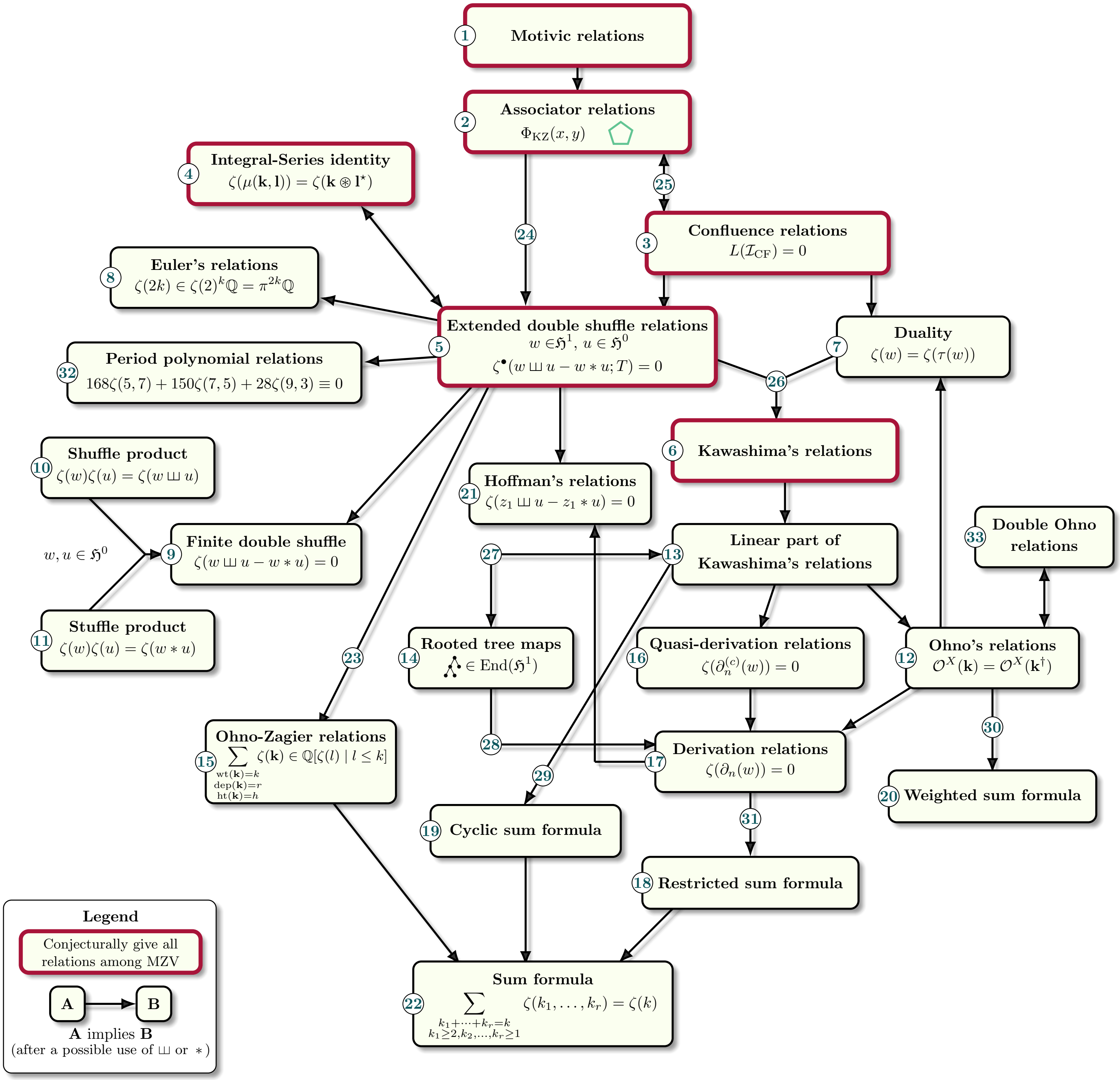


Figure 1: Overview of some relations among multiple zeta values.

(12) **Ohno's relations:** This is Theorem 3.13.

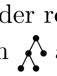
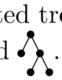
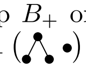
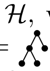
(13) **Linear part of Kawashima's relations** This is the $m = 1$ case of Theorem 3.19. Notice that in this case the sum on the left-hand side of (3.11) is zero and therefore we obtain the linear relation

$$\zeta(\varphi(v * w) \circledast y) = 0\,.$$

The number of relations obtained from the linear part of Kawashima's relations is given by the following table (calculated by Tanaka in [Tan2]).

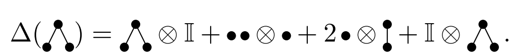
weight k	3	4	5	6	7	8	9	10	11	12
# all conjectured relations	1	3	6	14	29	60	123	249	503	1012
# Linear part of Kawashima's relations	1	2	5	10	23	46	98	200	413	838

(14) **Tanaka's rooted tree maps:** Rooted tree maps were introduced by Tanaka in [Tan3]. To a rooted tree he assigns a map $f \in \operatorname{End}\mathfrak{H}$, which gives an element in $f(w) \in \ker\zeta$, when evaluated at an admissible word $w \in \mathfrak{H}^0$. Before we can give the definition of the rooted tree maps, we need to recall some basics on rooted trees and the Connes-Kreimer coproduct.

A rooted tree is as a finite graph which is connected has no cycles, and has a distinguished vertex called the root. We draw rooted trees with the root on top, and we just consider rooted trees with no plane structure, which means that we, for example, do not distinguish between  and . A product (given by the disjoint union) of rooted trees will be called a (rooted) forest, and by $\mathcal{H}$ we denote the $\mathbb{Q}$-algebra of forests generated by all trees. The unit of $\mathcal{H}$, given by the empty forest, will be denoted by $\mathbb{I}$. Since we just consider trees without plane structure, the algebra $\mathcal{H}$ is commutative. Due to the work of Connes and Kreimer ([CK]), the space $\mathcal{H}$ has the structure of a Hopf algebra. To define the coproduct on $\mathcal{H}$, we first define the linear map B_+ on $\mathcal{H}$, which connects all roots of the trees in a forest to a new root. For example we have B_+  = . Clearly for every non-empty tree $t \in \mathcal{H}$ there exists a unique forest $f_t \in \mathcal{H}$ with $t = B_+(f_t)$, which is just given by removing the root of t. The coproduct on $\mathcal{H}$ can then be defined recursively for a tree $t \in \mathcal{H}$ by

$$\Delta(t) = t \otimes \mathbb{I} + (\mathrm{id} \otimes B_+) \circ \Delta(f_t)$$

and for a forest $f = gh$ with $g, h \in \mathcal{H}$ multiplicatively by $\Delta(f) = \Delta(g)\Delta(h)$ and $\Delta(\mathbb{I}) = \mathbb{I} \otimes \mathbb{I}$. For example we have



In [Tan3] Tanaka uses the coproduct Δ to assign to a forest $f \in \mathcal{H}$ a $\mathbb{Q}$-linear map on the space $\mathfrak{H}$, called a rooted tree map, by the following:

Definition 3.20. *The rooted tree map of the empty forest $\mathbb{I}$ is given by the identity map on $\mathfrak{H}$. For any non-empty forest $f \in \mathcal{H}$, we define a $\mathbb{Q}$-linear map on $\mathfrak{H}$, also denoted by f, recursively: For a word $w \in \mathfrak{H}$ and a letter $u \in \{x, y\}$ we set*

$$f(wu) := M(\Delta(f)(w \otimes u))\,, \tag{3.12}$$

where $M(w_1 \otimes w_2) = w_1 w_2$ denotes the multiplication on $\mathfrak{H}$. This reduces the calculation to $f(u)$ for a letter $u \in \{x, y\}$, which is defined by the following:

i) If $f = \bullet$, then $f(x) := xy$ and $f(y) := -xy$.

ii) For a tree $t = B_+(f)$ we set $t(u) := R_y R_{x+2y} R_y^{-1} f(u)$, where R_v is the linear map given by $R_v(w) = wv$ $(v, w \in \mathfrak{H})$.

iii) If $f = gh$ is a forest with $g, h \neq \mathbb{I}$, then $f(u) := g(h(u))$.

Theorem 3.21. *([Tan3, Theorem 1.3]) For any non-empty forest $f \in \mathcal{H}$ we have*

$$f(\mathfrak{H}^0) \subset \ker \zeta.$$

Example 3.22. *For the tree $f = \overset{\bullet}{\underset{\bullet}{|}}$ and the word $w = xy$ we obtain for $f(w)$*

$$\overset{\bullet}{\underset{\bullet}{|}}(xy) = M(\Delta(\overset{\bullet}{\underset{\bullet}{|}})(x \otimes y)) = M(\overset{\bullet}{\underset{\bullet}{|}}(x) \otimes y + \bullet(x) \otimes \bullet(y) + x \otimes \overset{\bullet}{\underset{\bullet}{|}}(y)).$$

Together with $\bullet(x) = xy$ and $\overset{\bullet}{\underset{\bullet}{|}}(x) = R_y R_{x+2y} R_y^{-1} \bullet(x) = x(x+2y)y$ we get

$$\overset{\bullet}{\underset{\bullet}{|}}(xy) = 2xyyy - xyxy - xxxy - xxyy = 2z_2 z_1 z_1 - z_2 z_2 - z_4 - z_3 z_1\,,$$

which by Theorem 3.21 gives the linear relation $2\zeta(2,1,1) = \zeta(4) + \zeta(2,2) + \zeta(3,1)$.

(15) **Ohno-Zagier relations:** We define the **height** of an index $\mathbf{k} = (k_1, \dots, k_j)$ by

$$\mathrm{ht}(\mathbf{k}) = \#\{i \mid k_i > 1\}\,,$$

i.e. the number of k_j not equal to 1. The Ohno-Zagier relations give an explicit formula for the sum of all multiple zeta values of a fixed weight, depth and height as a polynomial in single zeta values:

Theorem 3.23 ([OZ])**.** *We have*

$$\sum_{\substack{k \geq r+h \\ r \geq h \geq 1}} \Bigg(\sum_{\substack{\mathbf{k} \ adm. \\ \mathrm{wt}(\mathbf{k})=k \\ \mathrm{dep}(\mathbf{k})=r \\ \mathrm{ht}(\mathbf{k})=h}} \zeta(\mathbf{k}) \Bigg) X^{k-r-h} Y^{r-h} Z^{h-1} = \frac{1}{XY - Z} \left(1 - \exp\left(\sum_{n=2}^{\infty} \frac{\zeta(n)}{n} S_n(X,Y,Z) \right) \right)\,,$$

where the $S_n(X,Y,Z) \in \mathbb{Z}[X,Y,Z]$ are defined by

$$S_n(X,Y,Z) = X^n + Y^n - \alpha^n - \beta^n, \qquad \alpha, \beta = \frac{X + Y \pm \sqrt{(X+Y)^2 - 4Z}}{2}\,.$$

For $n = 2, \dots, 5$ the $S_n(X,Y,Z)$ are given by

$$\begin{aligned} &S_2(X,Y,Z) = -2XY + 2Z, \quad S_3(X,Y,Z) = -3X^2Y - 3XY^2 + 3XZ + 3YZ, \\ &S_4(X,Y,Z) = -4X^3Y - 6X^2Y^2 - 4XY^3 + 4X^2Z + 8XYZ + 4Y^2Z - 2Z^2\,. \end{aligned}$$

There are also Ohno-Zagier type relations for the q-MZV ζ_q^{BZ} proven by Okuda and Takeyama in [OT].

(16) **Quasi-derivation relations:** Quasi-derivation relations were first proposed in [Kan], and then it was shown in [Tan2] that they give linear relations among multiple zeta values.

Definition 3.24. *Let $c \in \mathbb{Q}$ and H the derivation on $\mathfrak{H}$ defined by $H(w) = \deg(w)w$ for any $w \in \mathfrak{H}$. For an integer $n \geq 1$, the $\mathbb{Q}$-linear map $\partial_n^{(c)} : \mathfrak{H} \to \mathfrak{H}$, called* **quasi-derivation***, is defined by*[7]

$$\partial_n^{(c)} = \frac{1}{(n-1)!} \operatorname{ad}\left(\theta^{(c)}\right)^{n-1} (\partial_1) \, ,$$

where $\theta^{(c)} : \mathfrak{H} \to \mathfrak{H}$ is the $\mathbb{Q}$-linear map defined by $\theta^{(c)}(x) = \frac{1}{2}(xz + zx)$, $\theta^{(c)}(y) = \frac{1}{2}(yz + zy)$ with $z = x + y$ and the rule

$$\theta^{(c)}(ww') = \theta^{(c)}(w)w' + w\theta^{(c)}(w') + c\partial_1(w)H(w')$$

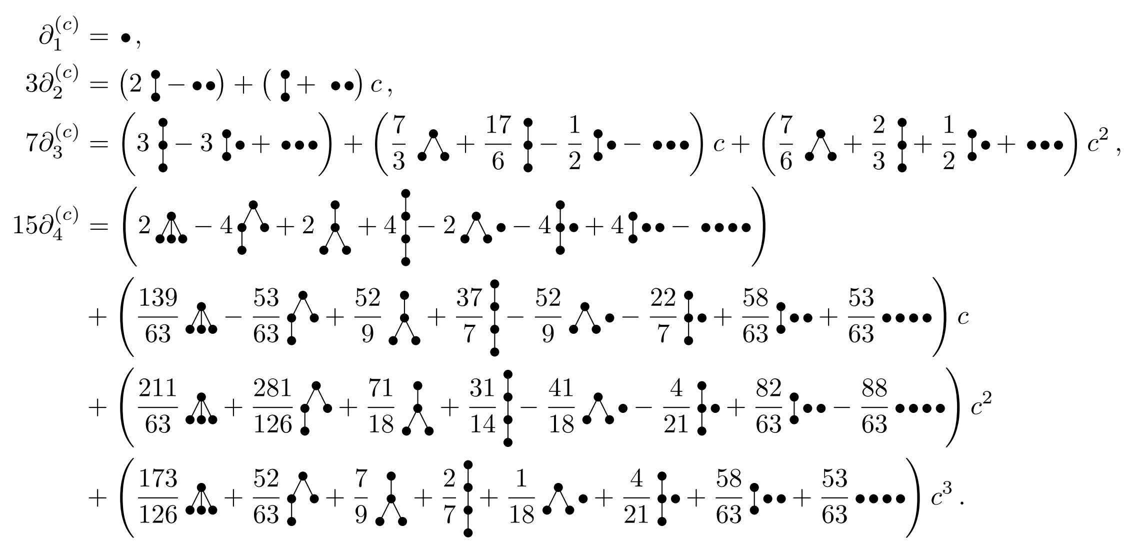
for any $w, w' \in \mathfrak{H}$.

In [Tan2] it was shown that $\partial_n^{(c)}$ evaluated at admissible words gives linear relations among multiple zeta values. Further, it was shown that these relations are consequences of the linear part of Kawashima's relations.

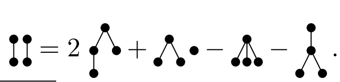
Theorem 3.25. *(Quasi-derivation relations, [Tan2, Theorem 3]) For all $n \geq 1$ and $c \in \mathbb{Q}$ we have*

$$\partial_n^{(c)}(\mathfrak{H}^0) \subset \ker \zeta \, .$$

Open problem 3.26. *Show that the quasi-derivations $\partial_n^{(c)}$ can be written in terms of rooted tree maps. In [BTan2] it was shown, that the linear part of the Kawashimas relation ($m = 1$ in Theorem 3.19) is equivalent to the rooted tree maps relations (Theorem 3.21). Since the proof ot the quasi-derivation relations just uses the linear part of the Kawashima's relations one might expect that there is an explicit relationsship. For $n = 1, 2, 3, 4$ one can actually show that we have*



But for $n \geq 5$ it is not clear how to express $\partial_n^{(c)}$ in terms of rooted tree maps and for $n \geq 4$ this representation is also not unique, since there are relations among rooted tree maps. For example we have



[7] Here $\operatorname{ad}(\theta)(\partial) := \theta\partial - \partial\theta$.

(17) **Derivation relations:** Define for $n \geq 1$ the derivation ∂_n on $\mathfrak{H}$ by $\partial_n(x) = x(x+y)^{n-1}y$ and $\partial_n(y) = -x(x+y)^{n-1}y$. This is a derivation on $\mathfrak{H}$ with respect to the usual non-commutative multiplication and therefore is suffices to just define it on the generators x and y. For any $w = uv$ with $u, v \in \mathfrak{H}$ it is then defined by using Leibniz's rule $\partial_n(uv) = \partial_n(u)v + u\partial_n(v)$.

Theorem 3.27. *(Derivation relation, [IKZ, Corollary 6]) For all $n \geq 1$ we have*

$$\partial_n(\mathfrak{H}^0) \subset \ker \zeta \,.$$

Also notice that this is the $c = 0$ case of the quasi-derivation relations (Theorem 3.25), since $\partial_n^{(0)} = \partial_n$.

Example 3.28. *If $n = 2$ we have*

$$\partial_2(x) = -\partial_2(y) = xxy + xyy \,,$$

i.e. we get for the admissible word xy:

$$\begin{aligned}\partial_2(xy) &= \partial_2(x)y + x\partial_2(y)\\ &= xxyy + xyyy - xxxy - xxyy = xyyy - xxxy = z_{2,1,1} - z_4 \,.\end{aligned}$$

The derivation relation then gives the relation $\zeta(2,1,1) = \zeta(4)$.

(18) **Restricted sum formula:** As a generalization of the sum formula Eie, Liaw, and Ong proved the following formula.

Theorem 3.29 (Restriced sum formula, [ELO])**.** *For integers $p \geq 0$ and $k > r \geq 1$ we have*

$$\sum_{\substack{\mathbf{k}\ adm.\\ \mathrm{wt}(\mathbf{k})=k\\ \mathrm{dep}(\mathbf{k})=r}} \zeta(\mathbf{k}, \{1\}^p) = \sum_{\substack{\mathbf{l}\ adm.\\ \mathrm{wt}(\mathbf{l})=k+p\\ \mathrm{dep}(\mathbf{l})=p+1\\ l_{p+1}>k-r+1}} \zeta(\mathbf{l}) \,.$$

Notice that this reduces to the sum formula (Theorem 3.12) in the case $p = 0$.

(19) **Cyclic sum formula:** In [HO] Hoffman and Ohno proved the following relation.

Theorem 3.30 (Cyclic sum formula)**.** *Let $k_1, \dots, k_r \geq 1$ be integers with at least one $k_j \geq 2$. Then*

$$\sum_{j=1}^{r} \zeta(k_j + 1, k_{j+1}, \dots, k_r, k_1, \dots, k_{j-1}) = \sum_{\substack{1\leq j\leq r\\ k_j\geq 2}} \sum_{m=0}^{k_j-2} \zeta(k_j - m, k_{j+1}, \dots, k_r, k_1, \dots, k_{j-1}, m+1) \,.$$

Example 3.31. *If we take $k_1 = 1, k_2 = 2$ and $k_3 = 3$ the cyclic sum formula gives*

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

(20) **Weighted sum formula:** There are different types of weighted sum formulas, and one variant of them can be, for example, found in [Kad].

(21) **Hoffman's relations:** This is Proposition 3.5.

(22) **Sum formula:** This is Theorem 3.12.

(23) **The extended double shuffle relations imply the Ohno-Zagier relations:** See [L].

(24) **The associator relations imply the extended double shuffle relations:** See [F2].

(25) **The associator relations and the confluence relations are equivalent:** See [F3].

(26) **The extended double shuffle relations together with the duality imply Kawashima's relations:** See [Kaw].

(27) **The rooted tree maps relations are equivalent to the linear part of Kawashima's relations:** See [BTan1].

(28) **The rooted tree maps relations imply the derivation relation:** This was shown in [BTan1] by writing the derivations ∂_n explicitly as rooted tree maps. For this just trees without any branches are needed, i.e. just consider for $m \geq 1$ the ladder trees

$$\lambda_m = \left.\begin{matrix}\bullet\\ \bullet\\ \vdots\\ \bullet\\ \bullet\end{matrix}\right\} m$$

and set $\lambda_0 = \mathbb{I}$. With this the main result of [BTan1] states.

Theorem 3.32 ([BTan1])**.** *For all $n \geq 1$ the derivation ∂_n is given by*

$$\partial_n = \frac{n}{2^n - 1} \sum_{d=1}^{n} \frac{(-1)^{d+1}}{d} \sum_{\substack{m_1+\dots+m_d=n\\ m_1,\dots,m_d \geq 1}} \lambda_{m_1} \dots \lambda_{m_d} \,. \tag{3.13}$$

By Definition 3.20 iii) we have $\lambda_{m_1}\lambda_{m_2} = \lambda_{m_2}\lambda_{m_1}$, so we get for the first few values of n ($w \in \mathfrak{H}$)

$$\partial_1(w) = \bullet(w)\,, \quad \partial_2(w) = \frac{2}{3}\substack{\bullet\\ \bullet}(w) - \frac{1}{3}\bullet\bullet(w)\,, \quad \partial_3(w) = \frac{3}{7}\substack{\bullet\\ \bullet\\ \bullet}(w) - \frac{3}{7}\substack{\bullet\\ \bullet}\bullet(w) + \frac{1}{7}\bullet\bullet\bullet(w)\,.$$

(29) **The linear part of Kawashima's relations imply the cyclic sum formula:** See [TW].

(30) **Ohno's relations imply the weighted sum formula:** See [Kad].

(31) **The derivation relations imply the restricted sum formula:** See [Tan4].

(32) **Period polynomial relations:** These types of relations will be explained in the next section (See Corollary 4.32 or [GKZ]).

(33) **Double Ohno relations** See [HMOS] and [HSS].

§4 Double zeta values and modular forms

In this section, we will focus on the extended double shuffle relations in the smallest depth, i.e., on some of the relations among double zeta values. Almost all results in this section are contained in or inspired by the work [GKZ].

4.1 The formal double zeta space

The idea of the formal double zeta space is to consider formal symbols, which satisfy the same relations as double zeta values, which come from the double shuffle relations in the smallest depths. We, therefore, start by recalling these relations before defining the formal double zeta space.

4.1.1 Double zeta values

Recall that for $k_1, k_2 \geq 2$ we have the finite double shuffle relations

$$\begin{aligned}\zeta(k_1)\zeta(k_2) &= \zeta(k_1,k_2) + \zeta(k_2,k_1) + \zeta(k_1+k_2)\\ &= \sum_{j=2}^{k_1+k_2-1}\left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1}\right)\zeta(j, k_1+k_2-j)\,.\end{aligned}$$

Using the stuffle and shuffle regularized multiple zeta values, we have for all $k_1, k_2 \geq 1$

$$\begin{aligned}\zeta^*(k_1;T)\zeta^*(k_2;T) &= \zeta^*(k_1,k_2;T) + \zeta^*(k_2,k_1;T) + \zeta^*(k_1+k_2;T)\\ &= \sum_{j=1}^{k_1+k_2-1}\left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1}\right)\zeta^{ш}(j, k_1+k_2-j;T)\,.\end{aligned} \tag{4.1}$$

The comparison map ρ (Theorem 2.35), which gives $\zeta^{ш}(\mathbf{k};T) = \rho(\zeta^{ш}(\mathbf{k};T))$, satisfies $\rho(1) = 1, \rho(T) = T$ and $\rho(T^2) = T^2 + \zeta(2)$. Therefore the $\zeta^{ш}(k_1,k_2;T)$ and $\zeta^*(k_1,k_2;T)$ just differ in the case $k_1 = k_2 = 1$ and we have

$$\zeta^{ш}(1,1;T) = \zeta^*(1,1;T) + \frac{1}{2}\zeta(2)\,, \tag{4.2}$$

and $\zeta^{ш}(1,1;T) = \frac{1}{2}T^2$, $\zeta^*(1,1;T) = \frac{1}{2}T^2 - \frac{1}{2}\zeta(2)$. Now define for $\bullet \in \{ш, *\}$ their generating series

$$\mathfrak{T}^\bullet(X) = \sum_{k\geq 1}\zeta^\bullet(k;T)X^{k-1}\,, \qquad \mathfrak{T}^\bullet(X,Y) = \sum_{k_1,k_2\geq 1}\zeta^\bullet(k_1,k_2;T)X^{k_1-1}Y^{k_2-1}\,.$$

Using $\frac{X^{k-1}-Y^{k-1}}{X-Y} = \sum_{k_1+k_2=k} X^{k_1-1}Y^{k_2-1}$ we see that (4.1) together with (4.2) can therefore be written as

$$\begin{aligned}\mathfrak{T}^\bullet(X)\mathfrak{T}^\bullet(Y) &= \mathfrak{T}^\bullet(X,Y) + \mathfrak{T}^\bullet(Y,X) + \frac{\mathfrak{T}^\bullet(X) - \mathfrak{T}^\bullet(Y)}{X-Y} - \delta_{\bullet,ш}\zeta(2)\\ &= \mathfrak{T}^\bullet(X+Y,Y) + \mathfrak{T}^\bullet(X+Y,X) + \delta_{\bullet,*}\zeta(2)\,,\end{aligned} \tag{4.3}$$

where δ denotes the Kronecker-delta.

4.1.2 The formal double zeta space

We will now define the formal double zeta space which is spanned by formal symbols Z_k, Z_{k_1,k_r} and P_{k_1,k_2} for $k, k_1, k_2 \geq 2$, which satisfy similar relations to the regularized versions of $\zeta(k), \zeta(k_1,k_2)$ and $\zeta(k_1)\zeta(k_2)$. The only difference will be, that we will ignore the correction term in the $k=2$ case, which will not bring any problems but makes things a little bit cleaner.

Definition 4.1. *We define for $k \geq 1$ the* **formal double zeta space** *in weight k as*

$$\mathcal{D}_k = \left\langle Z_k, Z_{k_1,k_2}, P_{k_1,k_2} \mid k_1+k_2=k, k_1,k_2 \geq 1 \right\rangle_{\mathbb{Q}} \Big/ (4.4)$$

where we divide out the following relations for $k_1, k_2 \geq 1$

$$\begin{aligned} P_{k_1,k_2} &= Z_{k_1,k_2} + Z_{k_2,k_1} + Z_{k_1+k_2} \\ &= \sum_{j=1}^{k_1+k_2-1} \left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1} \right) Z_{j,k_1+k_2-j}\,. \end{aligned} \tag{4.4}$$

Remark 4.2. Notice that by definition the P_{k_1,k_2} can always be expressed in terms of the Z and it would therefore be equivalent to define the space $\mathcal{D}_k$ by the span of elements Z_{k_1,k_2} and Z_k modulo the relations

$$Z_{k_1,k_2} + Z_{k_2,k_1} + Z_{k_1+k_2} = \sum_{j=1}^{k_1+k_2-1} \left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1} \right) Z_{j,k_1+k_2-j}\,. \tag{4.5}$$

But it is convenient to also work with the P_{k_1,k_2}, since they correspond to something like the product in most of the realizations (Definition 4.3) later.

For small weights the formal double zeta space is given by the following relations and basis elements. Since $P_{k_1,k_2} = P_{k_2,k_1}$ is symmetric we will always just consider the case $k_1 \leq k_2$.

k	Relations in $\mathcal{D}_k$	Basis of $\mathcal{D}_k$	$\dim_{\mathbb{Q}} \mathcal{D}_k$
1	-	Z_1	1
2	$Z_2 = 0, \quad P_{1,1} = 2Z_{1,1}$	$Z_{1,1}$	1
3	$Z_{2,1} = Z_3, \quad Z_{1,2} = P_{1,2} - 2Z_3$	$Z_3, P_{1,3}$	2
4	$Z_4 = 4Z_{3,1}, \quad Z_{2,2} = 3Z_{3,1},$ $P_{1,3} = Z_{1,3} + 5Z_{3,1}, \quad P_{2,2} = 10Z_{3,1}$	$Z_{1,3}, Z_{3,1}$	2
5	$Z_{4,1} = 2Z_5 - P_{2,3}, \quad Z_{3,2} = -\frac{11}{2}Z_5 + 3P_{2,3},$ $Z_{2,3} = \frac{9}{2}Z_5 - 2P_{2,3}, \quad Z_{1,4} = -3Z_5 + P_{1,4} + P_{2,3}$	$Z_5, P_{1,4}, P_{2,3}$	3
6	$Z_6 = 4Z_{3,3} + 4Z_{5,1}\,, \quad \ldots$	$Z_{1,5}, Z_{3,3}, Z_{5,1}$	3

Figure 2: Relations and bases for the formal double shuffle space in small weights.

Observe in Figure 2 that for even weight k we seem to have $\dim_{\mathbb{Q}} \mathcal{D}_k = \frac{k}{2}$ with a basis given by $Z_{\mathrm{odd,odd}}$ and for odd weight k it seems that $\dim_{\mathbb{Q}} \mathcal{D}_k = \frac{k+1}{2}$ with a basis given by Z_k and P_{k_1,k_2}. These observations are indeed correct and we will prove them in this section (Theorem 4.8 & 4.12). Notice that lower bounds of $\dim_{\mathbb{Q}} \mathcal{D}_k$, which coincides with the observed dimension, already follow from the definition. Since (4.5) is symmetric in k_1 and k_2 we obtain for k even $\frac{k}{2}$ relations among the k generators $Z_k, Z_{1,k}, \dots, Z_{k-1,1}$ and therefore we have for even k

$$\dim_{\mathbb{Q}} \mathcal{D}_k \geq \frac{k}{2}\,. \qquad (k \text{ even}) \tag{4.6}$$

For k odd we have $\frac{k-1}{2}$ relations and therefore

$$\dim_{\mathbb{Q}} \mathcal{D}_k \geq \frac{k+1}{2}\,. \qquad (k \text{ odd}) \tag{4.7}$$

It is convenient to consider generating series when working with the formal double zeta space and therefore we define the following elements in $\mathcal{D}_k[X,Y]$:

$$\begin{aligned}
\mathfrak{Z}_k(X,Y) &= \sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} Z_{k_1,k_2} X^{k_1-1} Y^{k_2-1}\,,\\
\mathfrak{P}_k(X,Y) &= \sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} P_{k_1,k_2} X^{k_1-1} Y^{k_2-1}\,,\\
\mathfrak{R}_k(X,Y) &= Z_k \frac{X^{k-1}-Y^{k-1}}{X-Y}\,.
\end{aligned}$$

With this the double shuffle relations (4.4) can be written as

$$\begin{aligned}
\mathfrak{P}_k(X,Y) &= \mathfrak{Z}_k(X,Y) + \mathfrak{Z}_k(Y,X) + \mathfrak{R}_k(X,Y)\\
&= \mathfrak{Z}_k(X+Y,Y) + \mathfrak{Z}_k(X+Y,X)\,.
\end{aligned} \tag{4.8}$$

We will not only be interested in relations in the space $\mathcal{D}_k$, but also in "real"-mathematical objects which satisfy these relations. Therefore we first introduce the following notation.

Definition 4.3. *Let A be a $\mathbb{Q}$-vector space. We define the* **A-valued points** *$\mathcal{D}_k(A)$ for $\mathcal{D}_k$ by*

$$\mathcal{D}_k(A) = \operatorname{Hom}_{\mathbb{Q}}(\mathcal{D}_k, A) = \left\{ (Z_k, Z_{k_1,k_2}) \in A^k \mid \text{ satisfying (4.5)} \right\}\,.$$

An element in $\mathcal{D}_k(A)$, i.e. one particular choice of $Z_k, Z_{k_1,k_2} \in A$ for all $k_1+k_2=k$ which satisfy (4.5)*, will be called a* **realization** *of the double zeta space in A.*

By comparing (4.3) and (4.8) we see that one realization is given by the shuffle regularized multiple zeta values: For $A = \mathbb{R}[T]$ a realization of $\mathcal{D}_k$ with $k \geq 1$ is given for $k_1, k_2 \geq 1$ and $k_1+k_2=k$ by

$$\begin{aligned}
Z_k &\longmapsto \begin{cases} \zeta^{ш}(k;T) & k \neq 2\\ 0 & k=2 \end{cases}\,,\\
Z_{k_1,k_2} &\longmapsto \zeta^{ш}(k_1,k_2;T)\,,\\
P_{k_1,k_2} &\longmapsto \zeta^{ш}(k_1;T)\zeta^{ш}(k_2;T)\,.
\end{aligned}$$

We will refer to this realization as the **multiple zeta realization**. Later we will also introduce realizations in the cases $A = \mathbb{Q}$, $A = \mathbb{Q}[[q]]$ and $A = \mathcal{O}(\mathbb{H})$. But before doing so we will prove some results in $\mathcal{D}_k$. Using the description in terms of generating series we obtain the following theorem.

Theorem 4.4. *i) For all $k \geq 2$ we have*

$$\sum_{j=2}^{k-1} Z_{j,k-j} = Z_k\,.$$

ii) For $k \geq 2$ even, we have

$$\sum_{\substack{j=2 \\ j \text{ even}}}^{k-2} Z_{j,k-j} = \frac{3}{4} Z_k\,, \qquad \sum_{\substack{j=2 \\ j \text{ odd}}}^{k-1} Z_{j,k-j} = \frac{1}{4} Z_k\,.$$

Proof. By (4.8) we have

$$D(X,Y) := \mathfrak{Z}_k(X+Y,Y) + \mathfrak{Z}_k(X+Y,X) - \mathfrak{Z}_k(X,Y) - \mathfrak{Z}_k(Y,X) - \mathfrak{R}_k(X,Y) = 0\,.$$

The first statement now follows by taking the case $(X,Y) = (1,0)$, since

$$0 = D(1,0) = \mathfrak{Z}_k(1,0) + \mathfrak{Z}_k(1,1) - \mathfrak{Z}_k(1,0) - \mathfrak{Z}_k(0,1) - Z_k = \sum_{j=1}^{k-1} Z_{j,k-j} - Z_{1,k-1} - Z_k\,.$$

For the second statement first consider for even k

$$0 = D(1,-1) = \mathfrak{Z}_k(0,-1) + \mathfrak{Z}_k(0,1) - \mathfrak{Z}_k(1,-1) - \mathfrak{Z}_k(-1,1) - Z_k = 2\sum_{j=2}^{k-1} (-1)^j Z_{j,k-j} - Z_k\,.$$

Taking $D(1,0) \pm \frac{1}{2} D(1,-1)$ we therefore obtain

$$\begin{aligned} 0 = D(1,0) + \frac{1}{2} D(1,-1) &= 2 \sum_{\substack{j=2 \\ j \text{ even}}}^{k-2} Z_{j,k-j} - \frac{3}{2} Z_k \\ 0 = D(1,0) - \frac{1}{2} D(1,-1) &= 2 \sum_{\substack{j=2 \\ j \text{ odd}}}^{k-1} Z_{j,k-j} - \frac{1}{2} Z_k\,, \end{aligned}$$

from which the second statement follows after dividing by 2. □

These polynomials are all elements in $\mathcal{D}_k \otimes_{\mathbb{Q}} V_k$, where $V_k \subset \mathbb{Q}[X,Y]$ denotes the space of all homogeneous polynomials of degree $k-2$. On V_k we define a right-action of $\mathrm{GL}_2(\mathbb{Z})$ for a $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{GL}_2(\mathbb{Z})$ and $F \in V_k$ by

$$(F|\gamma)(X,Y) = F(aX+bY, cX+dY)\,.$$

This action can then extended linearly to an action of the group ring $\mathbb{Z}[\mathrm{GL}_2(\mathbb{Z})]$ on $\mathcal{D}_k \otimes_{\mathbb{Q}} V_k$. The following elements in $\mathrm{GL}_2(\mathbb{Z})$ will be of importance when working with the above group action.

$$\begin{aligned} \sigma &= \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, & \epsilon &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \delta &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \\ T &= \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, & S &= \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, & U &= \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}. \end{aligned}$$

With this we can rewrite (4.8) even simpler as

$$\begin{aligned}\mathfrak{P}_k &= \mathfrak{Z}_k \,|(1+\epsilon) + \mathfrak{R}_k \\ &= \mathfrak{Z}_k \,|T(1+\epsilon)\,.\end{aligned} \tag{4.9}$$

Lemma 4.5. *For $k \geq 1$ and $A = \epsilon U \epsilon$ we have*

$$\mathfrak{Z}_k \mid (1-\sigma) = \mathfrak{P}_k \,|(1-\delta)(1+A-SA^2) - \mathfrak{R}_k \,|(1+A+A^2)\,.$$

Proof. First notice that $A = \epsilon U \epsilon = T\epsilon T^{-1}\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix}$ and that we have $A^3 = \sigma$. By (4.9) we get

$$\begin{aligned}\mathfrak{Z}_k \,|\epsilon &= -\mathfrak{Z}_k + \mathfrak{P}_k - \mathfrak{R}_k \\ \mathfrak{Z}_k \,|T\epsilon T^{-1} &= -\mathfrak{Z}_k + \mathfrak{P}_k \,|T^{-1}\,.\end{aligned}$$

and therefore

$$\mathfrak{Z}_k \,|A = \mathfrak{Z}_k \,|(T\epsilon T^{-1})\epsilon = \left(-\mathfrak{Z}_k + \mathfrak{P}_k \,|T^{-1}\right) |\epsilon = \mathfrak{Z}_k + \underbrace{\mathfrak{P}_k \,|(T^{-1}\epsilon - 1) + \mathfrak{R}_k}_{=:\mathfrak{K}}\,.$$

Iterating this identity two more times we get

$$\mathfrak{Z}_k \,|A^3 = \mathfrak{Z}_k + \mathfrak{K} \,|(1+A+A^2)\,.$$

By direct calculation one can check that the action of $(T^{-1}\epsilon - 1)(1+A+A^2)$ and $-(1-\delta)(1+A-SA^2)$ is the same on the symmetric polynomial $\mathfrak{P}_k$. □

Since $(\mathfrak{Z}_k \mid \sigma)(X,Y) = \mathfrak{Z}_k(-X,-Y) = (-1)^k \mathfrak{Z}_k(X,Y)$ we have

$$\mathfrak{Z}_k \mid (1-\sigma) = \begin{cases} 2\,\mathfrak{Z}_k & ,k \text{ odd} \\ 0 & ,k \text{ even}\,. \end{cases}$$

Also notice that $\mathfrak{P}_k \,|(1-\delta)$ is the generating series of $P_{\mathrm{ev},\dots}$, for which we write

$$\mathfrak{P}_k^{\mathrm{ev}}(X,Y) := \frac{1}{2}\left(\mathfrak{P}_k \,|(1-\delta)\right)(X,Y) = \sum_{\substack{j=2 \\ j \text{ even}}}^{k-1} P_{j,k-j} X^{j-1} Y^{k-j-1}\,.$$

Theorem 4.6 (Parity)**.** *For odd $k \geq 3$, every Z_{k_1,k_2} with $k_1, k_2 \geq 1$ and $k_1 + k_2 = k$ can be written as a linear combination of $P_{ev,od}$ and Z_k. More precisely we have*

$$Z_{k_1,k_2} = (-1)^{k_2} \sum_{\substack{j=2 \\ j\, even}}^{k-1} \left(\binom{k-j-1}{k_1-1} + \binom{k-j-1}{k_2-1} + (-1)^{k_2}\delta_{j,k_1} \right) P_{j,k-j} + \frac{1}{2}\left((-1)^{k_1}\binom{k_1+k_2}{k_2} - 1 \right) Z_k\,.$$

Proof. This follows directly from Lemma 4.5, by considering the coefficient of $X^{k_1-1}Y^{k_2-1}$ in

$$\mathfrak{Z}_k(X,Y) = \left(\mathfrak{P}_k^{\mathrm{ev}} \,|(1+A-SA^2)\right)(X,Y) - \frac{1}{2}\left(\mathfrak{R}_k \,|(1+A+A^2)\right)(X,Y)\,, \tag{4.10}$$

and checking that

$$\sum_{j=1}^{k-1} \left(\binom{k-j-1}{k_1-1} + \binom{k-j-1}{k_2-1} \right) = \binom{k_1+k_2}{k_1}\,.$$

□

Example 4.7. *As a consequence of Theorem 4.6 we get the following relations*

$$Z_{1,2} = P_{2,1} - 2Z_3\,, \qquad Z_{2,3} = -2P_{2,3} + \frac{9}{2}Z_5\,,$$
$$Z_{2,1} = Z_3\,, \qquad Z_{3,2} = 3P_{2,3} - \frac{11}{2}Z_5\,,$$
$$Z_{1,4} = P_{2,3} + P_{4,1} - 3Z_5\,, \qquad Z_{4,1} = -P_{2,3} + 2Z_5\,.$$

Using Theorem 4.6 we now can also prove the dimension formula for $\mathcal{D}_k$ in the odd weight k case.

Theorem 4.8. *For odd $k \geq 1$ we have $\dim_{\mathbb{Q}} \mathcal{D}_k = \frac{k+1}{2}$ and the sets*

$$B_1 = \{Z_k, P_{2,k-3}, P_{4,k-4}, \dots, P_{k-1,1}\}\,, \qquad B_2 = \{Z_k, Z_{1,k-1}, Z_{3,k-3}, \dots, Z_{k-2,2}\}\,,$$

are both bases of $\mathcal{D}_k$.

Proof. We already saw that $\dim_{\mathbb{Q}} \mathcal{D}_k \geq \frac{k+1}{2}$ since there are just $\frac{k-1}{2}$ different relations among the k generators of $\mathcal{D}$. To prove equality it suffices therefore to show that any element can be expressed in terms of elements in B_1 or B_2. By Theorem 4.6 we get that any element in $\mathcal{D}_k$ can be expressed as linear combinations of elements in B_1. For the second basis we just need to show, by symmetry, that any $P_{j,k-j}$ with j even can be expressed by Z_k and Z_{k_1,k_2} with k_1 odd. The equation in Theorem 4.6 modulo Z_k for odd $k_1 = 1, 3, \dots, k-2$ reads

$$Z_{k_1,k-k_1} \equiv -\sum_{\substack{j=2\\ j\,\text{even}}}^{k-1} \left(\binom{k-j-1}{k_1-1} + \binom{k-j-1}{k-k_1-1} \right) P_{j,k-j} \mod \mathbb{Q}Z_k\,.$$

We therefore need to show that the matrix $\left(\binom{k-2j-1}{2i-2} + \binom{k-2j-1}{k-2i} \right)_{1 \leq i,j \leq \frac{k-1}{2}}$ is invertible. The binomial coefficient $\binom{m}{n} = \frac{m}{n}\binom{m-1}{n-1}$ is even, when m is even and n is odd. Therefore modulo 2 the factor $\binom{k-2j-1}{k-2i}$ vanishes and we get a triangular matrix with 1 on the diagonal, from which we deduce that the matrix is invertible and therefore we can express $P_{j,k-j}$ in terms of $Z_{\text{odd,even}}$ and Z_k. □

4.1.3 The space $\mathcal{D}_k$ in even weight

We will now present consequences of Lemma 4.5 for the even weight case. In general the rest of the whole Section will be devoted to the even weight case and the connection to modular forms. For even k Lemma 4.5 implies relations among $P_{\text{ev,ev}}$ and Z_k.

Theorem 4.9 (Relations among $P_{\text{ev,ev}}$ and Z_{ev})**.** *For all $k_1, k_2 \geq 1$ with $k = k_1 + k_2$ even we have*

$$\frac{1}{2}\left(\binom{k_1+k_2}{k_2} - (-1)^{k_1} \right) Z_k = \sum_{\substack{j=2\\ j\,even}}^{k-2} \left(\binom{k-j-1}{k_1-1} + \binom{k-j-1}{k_2-1} - \delta_{j,k_1} \right) P_{j,k-j}\,. \tag{4.11}$$

Proof. This also follows from Lemma 4.5, considering the coefficient of $X^{k_1-1}Y^{k_2-1}$ in

$$\left(\mathfrak{P}_k^{\text{ev}} \mid (1 + A - SA^2) \right)(X,Y) = \frac{1}{2}\left(\mathfrak{R}_k \mid (1 + A + A^2) \right)(X,Y)\,. \tag{4.12}$$

□

Example 4.10. *As a consequence of Theorem 4.9 we get the following relations by considering the coefficients of* X^5Y *and* X^4Y^2 *in* (4.12)*:*

$$6P_{2,6} + 3P_{4,4} = \frac{27}{2} Z_8\,, \qquad 15P_{2,6} + 3P_{4,4} = \frac{57}{2} Z_8\,.$$

Combining these two relations we obtain

$$P_{4,4} = \frac{7}{6} Z_8\,.$$

Using the multiple zeta realization, this gives another proof of $\zeta(4)^2 = \frac{7}{6}\zeta(8)$*.*

Corollary 4.11. *For even* k *we have*

$$\sum_{\substack{j=2\\ j \text{ even}}}^{k-2} P_{j,k-j} = \frac{k+1}{2} Z_k\,.$$

Proof. This is the $(k_1, k_2) = (1, k-1)$ case in Theorem 4.9 but can also be obtained from the even sum formula in Theorem 4.4 ii) together with the relation $P_{j,k-j} = Z_{j,k-j} + Z_{k-j,j} + Z_k$. □

The even weight analogue of Theorem 4.8 is given by the following

Theorem 4.12. *For even* $k \geq 2$ *we have* $\dim_{\mathbb{Q}} \mathcal{D}_k = \frac{k}{2}$ *and the set of* $Z_{od,od}$*, i.e.*

$$\{Z_{1,k-1}, Z_{3,k-3}, \ldots, Z_{k-1,1}\}\,,$$

is a basis of $\mathcal{D}_k$*.*

Proof. We will give a proof of this below after introducing some further notation. Also, similar to the odd weight case, we will give explicit formulas to express the P_{k_1,k_2} and $Z_{\mathrm{ev,ev}}$ in terms of $Z_{\mathrm{od,od}}$, which can be found in (4.20). By Theorem 4.4 ii) this is already known for Z_k. □

Recall that by $V_k \subset \mathbb{Q}[X,Y]$ we denote the space of homogenous polynomials of degree $k-2$. In this section we just consider the case when k is even. In this case the action of $\mathrm{GL}_2(\mathbb{Z})$ from the previous section induces an action of $\Gamma := \mathrm{PGL}_2(\mathbb{Z})$ on V_k. On V_k we define the following pairing for $r, s, m, n \geq 1$, $r+s = m+n = k$

$$\langle X^{r-1}Y^{s-1}\,,\, X^{m-1}Y^{n-1}\rangle = \frac{(-1)^r}{\binom{k-2}{m-1}} \delta_{(r,s),(n,m)}\,. \tag{4.13}$$

Proposition 4.13. *i) For even* $k \geq 2$ *the pairing* (4.13) *on* V_k *is bilinear, symmetric and non-degenerated.*

ii) For even $k \geq 2$ *and* $F, G \in V_k$ *and* $\gamma \in \Gamma$ *we have*

$$\langle F|\gamma\,,\, G|\gamma\rangle = \langle F, G\rangle\,.$$

Proof. This is Exercise 13. □

Recall that we have $\mathfrak{Z}_k \,|(1+\epsilon) + \mathfrak{R}_k = \mathfrak{Z}_k \,|T(1+\epsilon)$. Defining the element

$$\Delta = (T-1)(\epsilon+1)$$

we see that this relation then is equivalent to $\mathfrak{Z}_k \,|\Delta = \mathfrak{R}_k$. Now denote for $\xi \in \mathbb{Z}[\mathrm{GL}_2(Z)]$ by ξ^* its adjoint action given by the anti-automorphism induced by $\gamma \mapsto \gamma^{-1}$. By the Γ invariance of the pairing we then obtain

$$\langle F|\xi \,,\, G\rangle = \langle F \,,\, G|\xi^*\rangle \,.$$

This means that for any $F \in V_k$ we get a relation in $\mathcal{D}_k$ with $\Delta^* = (1+\epsilon)(T^{-1}-1)$ by

$$\langle F|\,\Delta^* \,,\, \mathfrak{Z}_k\rangle = \langle F, \mathfrak{R}_k\rangle \,. \tag{4.14}$$

In the following we want to prove Theorem 4.12, i.e. show that any $Z_{\mathrm{ev,ev}}$ can be expressed in terms of $Z_{\mathrm{odd,odd}}$. To prove this we want to find for $m,n \geq 2$ polynomials $F_{m,n}(X,Y) \in V_{m+n}$ such that

$$F_{m,n} \,|\, (\Delta^* \pi^{\mathrm{od}}) \in X^{n-1} Y^{m-1} \mathbb{Q}^\times \,, \tag{4.15}$$

where $\pi^{\mathrm{od}} = \frac{1}{2}(1-\delta)$ is the projection to the odd part. This would imply that for some $\alpha_{k_1,k_2} \in \mathbb{Q}$ and $\lambda \in \mathbb{Q}^\times$ we have with $m+n=k$

$$\langle F_{m,n}|\,\Delta^* \,,\, \mathfrak{Z}_k\rangle = \lambda Z_{m,n} + \sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ odd}}} \alpha_{k_1,k_2} Z_{k_1,k_2} = \langle F_{m,n} \,,\, \mathfrak{R}_k\rangle \,, \tag{4.16}$$

which then gives an expression for $Z_{m,n}$ in terms of Z_k and $Z_{\mathrm{odd,odd}}$. We will deal with all $m,n \geq 2$ at the same time and therefore consider elements in

$$\mathcal{V}^{\mathrm{ev}} = \sum_{\substack{m\geq 2, n\geq 0\\ m,n \text{ even}}} V_{m+n}\, M^{m-2} N^n \subset \mathbb{Q}[[X,Y,M,N]] \,.$$

We extend the action of $\mathbb{Z}[\Gamma]$ to $\mathcal{V}^{\mathrm{ev}}$ and define the following element in $\mathcal{V}^{\mathrm{ev}}$

$$f_{M,N}(X,Y) := -\frac{1}{4} YN \cosh(MY) \left(\cosh(XN) \coth\left(\frac{YN}{2}\right) + \sinh(XN) \right) , \tag{4.17}$$

where

$$\cosh(X) = \sum_{\substack{n\geq 0\\ n \text{ even}}} \frac{X^n}{n!} \,, \quad \sinh(X) = \cosh'(X) = \sum_{\substack{n\geq 1\\ n \text{ odd}}} \frac{X^n}{n!}, \quad \frac{X}{2} \coth\left(\frac{X}{2}\right) = -\sum_{n\geq 1} \frac{B_n}{2n!} X^n \,.$$

With this we define the polynomials $F_{m,n}(X,Y) \in V_{m+n}$ for $m \geq 2, n \geq 0$ by

$$\begin{aligned} F_{M,N}(X,Y) &:= \sum_{\substack{m\geq 2, n\geq 0\\ m,n \text{ even}}} F_{m,n}(X,Y) \frac{M^{m-2}}{(m-2)!} \frac{N^n}{n!} \\ &:= f_{M,N}(X,Y) + f_{M,N}(Y,X) - f_{M,N}(-X, X+Y) \,, \end{aligned}$$

where the right-hand side is exactly $f_{M,N} \mid (1+\epsilon-ST)$. These $F_{m,n}$ give a solution to (4.15):

Lemma 4.14. *We have*

$$(F_{M,N} \,|\, (\Delta^* \pi^{od}))(X,Y) = NY \cosh(MY) \sinh(NX) = \sum_{\substack{m,n \geq 2 \\ m,n \text{ even}}} n X^{n-1} Y^{m-1} \frac{M^{m-2}}{(m-2)!} \frac{N^n}{n!}\,,$$

i.e. we have for even $m, n \geq 2$

$$F_{m,n} \,|\, (\Delta^* \pi^{od}) = n X^{n-1} Y^{m-1}\,.$$

Proof. This follows by a direct (but tedious) calculation using trigonometric identities. □

Using (4.16) this gives explicit expressions for $Z_{\mathrm{ev,ev}}$, which is given by the following.

Proposition 4.15. *For* $m, n \geq 2$ *even and* $k = m + n$ *we have*

$$Z_{m,n} = \frac{2}{1-m} \sum_{\substack{k_1+k_2=k \\ k_1,k_2 \geq 1 \text{ odd}}} \left(\sum_{j=0}^{\min\{k_1-2,n\}} \binom{k-2-j}{m-2} \binom{k_1-1}{j} B_{n-j} \right) \left(Z_{k_1,k_2} + \frac{1}{2} Z_k \right) - \frac{1}{2} Z_k\,.$$

Proof. By Lemma 4.14 the polynomials $F_{m,n}$ give the relation

$$\langle F_{m,n} | \, \Delta^*\,,\, \mathfrak{Z}_k \rangle = \frac{n(-1)^n}{\binom{k-2}{m-2}} Z_{m,n} + \sum_{\substack{k_1+k_2=k \\ k_1,k_2 \text{ odd}}} \alpha_{k_1,k_2} Z_{k_1,k_2} = \lambda Z_k\,, \tag{4.18}$$

where the coefficients $\alpha_{k_1,k_2} \in \mathbb{Q}$ and $\lambda = \langle F_{m,n}\,,\, \mathfrak{R}_k \rangle$ can be obtained by considering the coefficients of the generating series $F_{M,N}$. The same formula can also be found in [GKZ, (7)]. □

Clearly Proposition 4.15 also gives formulas for $P_{k_1,k_2} = Z_{k_1,k_2} + Z_{k_2,k_1} + Z_k$ in terms of $Z_{\mathrm{od,od}}$. For this we can define for even $m, n \geq 2$ and odd $k_1, k_2 \geq 1$ with $k_1 + k_2 = m + n$ the coefficients

$$\begin{aligned} \alpha^{m,n}_{k_1,k_2} &= \frac{2}{1-m} \sum_{j=0}^{\min\{k_1-2,n\}} \binom{k-2-j}{m-2} \binom{k_1-1}{j} B_{n-j}\,, \\ \lambda_{m,n} &= -\frac{1}{2} + \frac{1}{2} \sum_{\substack{k_1+k_2=k \\ k_1,k_2 \geq 1 \text{ odd}}} \alpha^{m,n}_{k_1,k_2}\,. \end{aligned} \tag{4.19}$$

From the odd/odd sum formula in Theorem 4.4 ii) we therefore get for even $m, n \geq 2$ the following two explicit formulas

$$\begin{aligned} Z_{m,n} &= \sum_{\substack{k_1+k_2=k \\ k_1 \geq 3, k_2 \geq 1 \text{ odd}}} \left(\alpha^{m,n}_{k_1,k_2} + 4\lambda_{m,n} \right) Z_{k_1,k_2}\,, \\ P_{m,n} &= \sum_{\substack{k_1+k_2=k \\ k_1 \geq 3, k_2 \geq 1 \text{ odd}}} \left(\alpha^{m,n}_{k_1,k_2} + \alpha^{n,m}_{k_1,k_2} + 4\lambda_{m,n} + 4\lambda_{n,m} + 4 \right) Z_{k_1,k_2}\,. \end{aligned} \tag{4.20}$$

This proofs Theorem 4.12], i.e. that the $Z_{\mathrm{od,od}}$ form a basis for the space $\mathcal{D}_k$ when k is even.

4.2 Realizations in $\mathbb{Q}$-algebras & Combinatorial double Eisenstein series

From now on we will be interested in realizations in a $\mathbb{Q}$-algebra A and we will consider all weights k at the same time. Assume we have a family homomorphism $\varphi = (\varphi_k)_{k\geq 1}$ where φ_k is a realization of $\mathcal{D}_k$ in A, i.e. $\varphi_k \in \mathrm{Hom}_{\mathbb{Q}}(\mathcal{D}_k, A)$. Such a family φ will be called a **realization of $\mathcal{D}$ in** A. For a realization φ we will write $\varphi(Z_{k_1,k_2}), \varphi(Z_{k_1,k_2})$ and $\varphi(Z_k)$ instead of $\varphi_{k_1+k_2}(P_{k_1,k_2}), \varphi_{k_1+k_2}(Z_{k_1,k_2}), \varphi_k(Z_k)$, since the weight is always clear from the indices.

Lemma 4.16. *Assume we have power series $P(X,Y), Z(X,Y), Z(X) \in A[[X,Y]]$ such that*

$$\begin{aligned} P(X,Y) &= Z(X,Y) + Z(Y,X) + \frac{Z(X)-Z(Y)}{X-Y} - z(2) \\ &= Z(X+Y,Y) + Z(X+Y,X)\,, \end{aligned}$$

where $Z(X) = \sum_{k\geq 1} z(k) X^{k-1}$. Then φ defined by

$$\begin{aligned} \varphi(Z_k) &= z(k) - \delta_{k,2} z(2)\,, \\ \varphi(Z_{k_1,k_2}) &= \textit{coefficient of } X^{k_1-1}Y^{k_2-1} \textit{ in } Z(X,Y)\,, \\ \varphi(P_{k_1,k_2}) &= \textit{coefficient of } X^{k_1-1}Y^{k_2-1} \textit{ in } P(X,Y) \end{aligned}$$

gives a realization of $\mathcal{D}$ in A.

Proof. This is the same argument as we had before for the realization φ_ζ given by shuffle regularized multiple zeta values. □

Theorem 4.17. *Let φ be a realization of $\mathcal{D}$ in an $\mathbb{Q}$-algebra A. For $k \geq 1$ we write*

$$\mathsf{Z}(k) = \varphi(Z_k) + \delta_{k,2}\mathsf{Z}(2)\,.$$

for some fixed element $\mathsf{Z}(2) \in A$.

i) Assume that for even $k_1, k_2 \geq 2$ we have

$$\varphi(P_{k_1,k_2}) = \mathsf{Z}(k_1)\mathsf{Z}(k_2)\,.$$

Then for even $k \geq 2$ we have $\mathsf{Z}(k) \in \mathbb{Q}[\mathsf{Z}(2)]$ and more precisely we obtain for $m \geq 1$

$$\mathsf{Z}(2m) = -\frac{B_{2m}}{2(2m)!}\left(-24\mathsf{Z}(2)\right)^m\,. \tag{4.21}$$

ii) Assume that there exist a derivation $\partial \in \mathrm{Der}(A)$ such that for all even $k_1, k_2 \geq 2$

$$\varphi(P_{k_1,k_2}) = \mathsf{Z}(k_1)\mathsf{Z}(k_2) + \frac{\delta_{k_1,2}}{2k_2}\,\partial\mathsf{Z}(k_2) + \frac{\delta_{k_2,2}}{2k_1}\,\partial\mathsf{Z}(k_1)\,.$$

Then for even $k \geq 2$ we have $\mathsf{Z}(k) \in \mathbb{Q}[\mathsf{Z}(2),\mathsf{Z}(4),\mathsf{Z}(6)]$. Moreover we get

$$\begin{aligned} \partial\mathsf{Z}(2) &= 5\,\mathsf{Z}(4) - 2\,\mathsf{Z}(2)^2\,, \\ \partial\mathsf{Z}(4) &= 8\,\mathsf{Z}(6) - 14\,\mathsf{Z}(2)\mathsf{Z}(4)\,, \\ \partial\mathsf{Z}(6) &= \frac{120}{7}\mathsf{Z}(4)^2 - 12\mathsf{Z}(2)\mathsf{Z}(6)\,, \\ \partial^3\mathsf{Z}(2) &= 36(\partial\mathsf{Z}(2))^2 - 24\mathsf{Z}(2)\partial^2\mathsf{Z}(2)\,, \end{aligned} \tag{4.22}$$

and therefore the space $\mathbb{Q}[\mathsf{Z}(2),\mathsf{Z}(4),\mathsf{Z}(6)] = \mathbb{Q}[\mathsf{Z}(2),\partial\mathsf{Z}(2),\partial^2\mathsf{Z}(2)]$ is closed under ∂.

iii) Assume that for even $k_1, k_2 \geq 4$

$$\varphi(P_{k_1,k_2}) = \mathsf{Z}(k_1)\mathsf{Z}(k_2)\,.$$

Then for even $k \geq 4$ we have $\mathsf{Z}(k) \in \mathbb{Q}[\mathsf{Z}(4), \mathsf{Z}(6)]$.

Proof. We first show ii). The explicit formulas in (4.22) can be obtained by combining the relations coming from Theorem 4.9 in the correct way. One of these relations (Corollary 4.11) gives for $k \geq 4$

$$\mathsf{Z}(k) = \frac{2}{k+1} \sum_{\substack{j=2 \\ j \text{ even}}}^{k-2} \varphi(P_{j,k-j}) = \frac{2}{k+1} \sum_{\substack{j=2 \\ j \text{ even}}}^{k-2} \mathsf{Z}(j)\mathsf{Z}(k-j) + \frac{2}{(k+1)(k-2)} \partial \mathsf{Z}(k-2)\,.$$

Inductively we see, together with (4.22), that $\mathsf{Z}(k) \in \mathbb{Q}[\mathsf{Z}(2), \mathsf{Z}(4), \mathsf{Z}(6)]$. The first statement in i) is just a special case of ii) for $\partial \equiv 0$. The explicit formula (4.21) can be obtained by considering the generating series of the right hand side and show that it satisfies the same recursion as the generating series of the left hand side (Exercise 12). For iii) consider the equation (4.11) in the cases $(k_1, k_2) = (m, 2)$ and $(k_1, k_2) = (m-1, 3)$. Taking $(m-1)$-times the first case and subtracting 2-times the second gives for even $k = m+2 \geq 8$ a relation of Z_k as a linear combination of $P_{j,k-j}$ with $j, k-j \geq 4$ even. Recursively it follows that $\mathsf{Z}(k) \in \mathbb{Q}[\mathsf{Z}(4), \mathsf{Z}(6)]$. □

Since the multiple zeta realiziation gives a realization of $\mathcal{D}$ in $\mathbb{R}$ which satisfies the condition in $i)$ with $\mathsf{Z}(2) = \zeta(2) = -\frac{(2\pi i)^2}{24}$, we obtain from (4.21) the Euler relation $\zeta(2m) = -\frac{B_{2m}}{2(2m)!}(2\pi i)^{2m}$.
The first three equations in (4.22) are known as **Ramanujan's differential equation** and the last one is called **Chazy equation** (e.g. see [Za2, Section 5.1]). One set of solutions for (4.21) (and actually a description of almost all solutions for the Chazy equation) is given by the Eisenstein series $\mathsf{Z}(k) = G_k$, which we defined for $k \geq 1$ by

$$G_k = -\frac{B_k}{2k!} + \mathrm{g}(k) = \beta(k) + \mathrm{g}(k)\,.$$

In the following, we want to introduce a realization, which satisfies the condition in ii), and which is exactly given by the Eisenstein series in depth one. For this we will first introduce a realization with $\mathsf{Z}(k) = \mathrm{g}(k)$ and then a realization with $\mathsf{Z}(k) = \beta(k)$. Since $\mathrm{Hom}_{\mathbb{Q}}(\mathcal{D}_k, A)$ are groups, we can add realizations and obtain another realization. Combining the above two realizations will then give us the realization of the Eisenstein series. We will see that this realization satisfies the conditions of ii) & iii) in Theorem 4.17 and therefore we will obtain a proof of (4.21) for Eisenstein series and the fact that every Eisenstein series G_k with $k \geq 4$ even can be written as a polynomial in G_4 and G_6.

4.2.1 Combinatorial double Eisenstein series

In this section we want to introduce a realization φ_G of $\mathcal{D}$ in the $\mathbb{Q}$-algebra $A = \mathbb{Q}[[q]]$, which is given by the Eisenstein series $G(k) = \beta(k) + \mathrm{g}(k)$ in depth one. As mentioned before we will introduce two realizations, one for the constant term, denoted by φ_β, and one for the "g-part", denoted by φ_{g}. The combinatorial double Eisenstein realization will then be their sum

$$\varphi_G = \varphi_\beta + \varphi_{\mathrm{g}}\,.$$

We will start with the realization φ_{g}, which in depth one will be given by $\varphi_{\mathrm{g}}(Z_k) = \mathrm{g}(k)$ for $k \neq 2$. To use Lemma 4.16 we need to consider their generating, which were defined in Section 1.4 by

$$\mathfrak{g}(X_1, \ldots, X_r) = \sum_{k_1,\ldots,k_r \geq 1} \mathrm{g}(k_1, \ldots, k_r) X_1^{k_1-1} \cdots X_r^{k_r-1}\,.$$

In Lemma 1.25 we saw that we have the following two explicit expressions

$$\begin{aligned}\mathfrak{g}(X_1,\dots,X_r) &= \sum_{m_1>\dots>m_r>0} \frac{e^{X_1}q^{m_1}}{1-e^{X_1}q^{m_1}}\cdots\frac{e^{X_r}q^{m_r}}{1-e^{X_r}q^{m_r}} \\ &= \sum_{m_1>\dots>m_r>0} \frac{e^{m_1X_r}q^{m_1}}{1-q^{m_1}}\frac{e^{m_2(X_{r-1}-X_r)}q^{m_2}}{1-q^{m_2}}\cdots\frac{e^{m_r(X_1-X_2)}q^{m_r}}{1-q^{m_r}}\,.\end{aligned} \tag{4.23}$$

To express their product in a suitable way we introduce the following series

$$\mathfrak{b}(X) = \frac{1}{2}\left(\frac{1}{X}-\frac{1}{e^X-1}-\frac{1}{2}\right) = \sum_{k\geq 1}\beta(k)X^{k-1} = -\sum_{k\geq 2}\frac{B_k}{2k!}X^{k-1} = \sum_{m\geq 1}\frac{\zeta(2m)}{(2\pi i)^{2m}}X^{2m-1}\,,$$

which will also give the depth one part of the realization φ_β.

Lemma 4.18. *We have*

$$\begin{aligned}\mathfrak{g}(X)\mathfrak{g}(Y) =\ & \mathfrak{g}(X,Y)+\mathfrak{g}(Y,X)+\frac{\mathfrak{g}(X)-\mathfrak{g}(Y)}{X-Y}+\Big(\mathfrak{b}(Y-X)-\mathfrak{b}(X-Y)\Big)\left(\mathfrak{g}(X)-\mathfrak{g}(Y)\right)-\frac{1}{2}\left(\mathfrak{g}(X)+\mathfrak{g}(Y)\right) \\ =\ & \mathfrak{g}(X+Y,X)+\mathfrak{g}(X+Y,Y)-\mathfrak{g}(X+Y)+(X+Y)\mathfrak{g}'(X+Y)+\mathrm{g}(2)\,,\end{aligned}$$

where we write $\mathfrak{g}'(X) = q\frac{d}{dq}\sum_{k\geq 1}\mathrm{g}(k)\frac{X^{k-1}}{k}$.

Proof. In Proposition 1.33 we showed by using (4.23) that

$$\begin{aligned}\mathfrak{g}(X)\mathfrak{g}(Y) &= \mathfrak{g}(X,Y)+\mathfrak{g}(Y,X)+\frac{1}{e^{X-Y}-1}\mathfrak{g}(X)+\frac{1}{e^{Y-X}-1}\mathfrak{g}(Y) \\ &= \mathfrak{g}(X+Y,X)+\mathfrak{g}(X+Y,Y)-\mathfrak{g}(X+Y)+q\frac{d}{dq}\sum_{k\geq 1}\mathrm{g}(k)\frac{(X+Y)^k}{k}+\mathrm{g}(2)\,,\end{aligned}$$

from which the statement follows by using the definition of $\mathfrak{b}(X)$. □

Theorem 4.19. *Define the following generating series*

$$\begin{aligned}\mathfrak{h}(X,Y) = \mathfrak{g}(X,Y) &- \left(\mathfrak{b}(X-Y)+\frac{1}{2}\right)\mathfrak{g}(X)+\mathfrak{b}(Y)\mathfrak{g}(X)+\mathfrak{b}(X-Y)\mathfrak{g}(Y) \\ &+\frac{1}{2}(X-Y)\mathfrak{g}'(Y)+\frac{1}{2}X\mathfrak{g}'(X)+\frac{1}{2}\,\mathrm{g}(2)\,,\end{aligned}$$

where as before $\mathfrak{g}'(X) = q\frac{d}{dq}\sum_{k\geq 1}\mathrm{g}(k)\frac{X^{k-1}}{k}$. *Then we have*

$$\begin{aligned}P(X,Y) &= \mathfrak{h}(X,Y)+\mathfrak{h}(Y,X)+\frac{\mathfrak{g}(X)-\mathfrak{g}(Y)}{X-Y}-\mathrm{g}(2) \\ &= \mathfrak{h}(X+Y,Y)+\mathfrak{h}(X+Y,X)\,,\end{aligned} \tag{4.24}$$

where

$$P(X,Y) = \mathfrak{g}(X)\mathfrak{g}(Y)+\mathfrak{b}(X)\mathfrak{g}(Y)+\mathfrak{b}(Y)\mathfrak{g}(X)+\frac{1}{2}\left(\mathfrak{g}'(X)Y+\mathfrak{g}'(Y)X\right)\,.$$

In particular (4.24) *gives a realization* φ_{g} *of* $\mathcal{D}$ *in* $q\mathbb{Q}[[q]]$ *by Lemma 4.16.*

Proof. This follows by a direct calculation from Lemma 4.18 but is also given in [GKZ, Theorem 7]. $\square$

We will now give the realization φ_β, which will give the constant term for the combinatorial double Eisenstein series.

Theorem 4.20. *With* $\mathfrak{b}(X) = \sum_{k\geq 1} \beta(k) X^{k-1} = \frac{1}{2}\left(\frac{1}{X} - \frac{1}{e^X-1} - \frac{1}{2}\right)$ *and*

$$\mathfrak{b}(X,Y) = \sum_{k_1,k_2\geq 1} \beta(k_1,k_2) X^{k_1-1} Y^{k_2-1}$$
$$:= \frac{1}{3}\big(\mathfrak{b}(X) + \mathfrak{b}(X-Y)\big)\mathfrak{b}(Y) - \frac{5}{12}\frac{\mathfrak{b}(X)-\mathfrak{b}(Y)}{X-Y} + \frac{\mathfrak{b}(X)-\mathfrak{b}(X-Y)}{4Y} - \frac{\mathfrak{b}(Y)-\mathfrak{b}(Y-X)}{12X} - \frac{1}{96}$$

we have

$$\begin{aligned}\mathfrak{b}(X)\mathfrak{b}(Y) &= \mathfrak{b}(X,Y) + \mathfrak{b}(Y,X) + \frac{\mathfrak{b}(X)-\mathfrak{b}(Y)}{X-Y} - \beta(2)\\ &= \mathfrak{b}(X+Y,Y) + \mathfrak{b}(X+Y,X)\,.\end{aligned}$$

In particular this gives a realization φ_β *of* $\mathcal{D}$ *in* $\mathbb{Q}$ *by Lemma 4.16.*

Proof. Again this can be checked explicitly by using the definition of $\mathfrak{b}(X)$. A more systematic point of view, which we will make more explicit later, is that the hyperbolic cotangent

$$F(X) = -\frac{1}{2}\frac{1}{X} + \mathfrak{b}(X) = -\frac{1}{4}\coth\left(\frac{X}{2}\right)$$

satisfies the Fay identity

$$F(X)F(Y) + F(X-Y)F(X) + F(-Y)F(X-Y) = \frac{1}{16}\,. \tag{4.25}$$

Writing $G(X,Y) = F(X)F(Y)$ the equation (4.25) can be written as $G \mid (1+U+U^2) = \frac{1}{16}$, which leads to a connection of period polynomials for modular forms. We will see later that basically any such G gives rise to a realization of $\mathcal{D}$ (Theorem 4.40). $\square$

Definition 4.21. *i) We define the* **combinatorial Eisenstein realization** *of* $\mathcal{D}$ *in* $\mathbb{Q}[[q]]$ *by*

$$\varphi_G = \varphi_\beta + \varphi_{\mathrm{g}}\,,$$

where the realization φ_β *and* φ_{g} *are given by Theorem 4.19 and 4.20.*

ii) For $k_1,k_2\geq 1$ *the* **combinatorial double Eisensteins series** $G(k_1,k_2)\in\mathbb{Q}[[q]]$ *are defined by* $G(k_1,k_2) = \varphi_G(Z_{k_1,k_2})$, *i.e. they are explicitly given by*

$$\sum_{k_1,k_2\geq 1} G(k_1,k_2) X^{k_1-1}Y^{k_2-1} := \mathfrak{b}(X,Y) + \mathfrak{h}(X,Y)\,,$$

where $\mathfrak{b}(X,Y)$ *and* $\mathfrak{h}(X,Y)$ *are given in Theorem 4.19 and 4.20.*

Notice that we have

$$\begin{aligned}\varphi_G(P_{k_1,k_2}) &= \beta(k_1,k_2) + \mathrm{g}(k_1)\,\mathrm{g}(k_2) + \beta(k_1)\,\mathrm{g}(k_2) + \beta(k_2)\,\mathrm{g}(k_1) + \frac{\delta_{k_1,2}}{2k_2} q\frac{d}{dq}\,\mathrm{g}(k_2) + \frac{\delta_{k_2,2}}{2k_1} q\frac{d}{dq}\,\mathrm{g}(k_1)\\ &= G_{k_1}G_{k_2} + \frac{\delta_{k_1,2}}{2k_2} q\frac{d}{dq} G_{k_2} + \frac{\delta_{k_2,2}}{2k_1} q\frac{d}{dq} G_{k_1}\,,\end{aligned}$$

and therefore the combinatorial Eisenstein realization satisfies the conditions for ii) with $\partial = q\frac{d}{dq}$ and iii) in Theorem 4.17. This gives a proof of Ramanujan's differential equations and the fact that for any even $k \geq 4$ we have $G_k \in \mathbb{Q}[G_4, G_6]$.

Proposition 4.22. *The combinatorial double Eisenstein series are modified q-analogues of the double zeta values, i.e. for $k_1 \geq 2, k_2 \geq 1$ we have*

$$\lim_{q \to 1} (1-q)^{k_1+k_2} G(k_1, k_2) = \zeta(k_1, k_2)\,.$$

Proof. This will be proven later when considering the q-series and their derivatives in more detail. □

Proposition 4.23. *Any modular form with rational coefficients can be written as a linear combination of $G(odd, odd)$, i.e for even $k \geq 4$ we have*

$$\mathcal{M}_k^{\mathbb{Q}} \subset \langle G(j, k-j) \mid j = 3, 5, \dots, k-1 \rangle_{\mathbb{Q}}\,.$$

Proof. This follows from the fact that any modular form can be written as a linear combination of products of Eisenstein series (Theorem 1.19) together with the explicit formulas for P_{k_1,k_2} in (4.20). □

Lemma 4.24. *For even $k \geq 4$ the set*

$$\{G_k\} \cup \left\{ G_{2j} G_{k-2j} \mid \left\lfloor \frac{k-2}{6} \right\rfloor + 2 \leq j \leq \left\lfloor \frac{k}{4} \right\rfloor \right\}$$

forms a basis of $\mathcal{M}_k^{\mathbb{Q}}$.

Proof. This is Corollary 1 in [HST]. □

By the Lemma we get a basis of $S_k^{\mathbb{Q}}$ by

$$\left\{ G_{2j} G_{k-2j} - \frac{\beta(2j)\beta(k-2j)}{\beta(k)} G_k \mid \left\lfloor \frac{k-2}{6} \right\rfloor + 2 \leq j \leq \left\lfloor \frac{k}{4} \right\rfloor \right\}.$$

Since we have for $k_1, k_2 \geq 4$ that $\varphi_G(P_{k_1,k_2}) = G_{k_1} G_{k_2}$ we can use an explicit version of Theorem 4.12 to give explicit expressions of this basis in terms of $G(\mathrm{odd}, \mathrm{odd})$. Using Proposition 4.22 and the fact that modular forms are also modified q-analogues of their constant terms gives us then an explanation for the factor $\mathsf{O}(X)\,\mathsf{O}(X) - \mathsf{S}(X)$ in the Broadhurst-Kreimer conjecture (Conjecture 1.21). Using the formulas for P_{k_1,k_2} in (4.20) one can therefore obtain an explicit basis of $S_k^{\mathbb{Q}}$ in terms of $G(\mathrm{odd}, \mathrm{odd})$.

Example 4.25. *i) A basis for $S_{12}^{\mathbb{Q}}$ is given by*

$$G(3,9) - \frac{23825}{5197} G(5,7) - \frac{41431}{10394} G(7,5) + \frac{360}{5197} G(9,3) + G(11,1)\,.$$

ii) A basis for $S_{16}^{\mathbb{Q}}$ is given by

$$G(3,13) - \frac{279116 G(5,11)}{78967} - \frac{2125607 G(7,9)}{315868} - \frac{154671 G(9,7)}{22562} - \frac{1040507 G(11,5)}{315868} + \frac{38573 G(13,3)}{157934} + G(15,1)\,.$$

4.3 Period polynomials

In this section, we will introduce period polynomials and their connection to relations in the formal double zeta space. Period polynomials are polynomials with complex coefficients associated to modular forms. Due to works of Eichler, Shimura, Manin, and Zagier, the spaces of period polynomials are isomorphic to the space of modular forms (For more details on this topic see [La], [Za4]). In this whole section we will always assume that k is even.

For a cusp for $f \in S_k$ we define its **period polynomial** as the following polynomial in $\mathbb{C} \otimes V_k$

$$P_f(X,Y) = \int_0^{i\infty} (X - Y\tau)^{k-2} f(\tau)\, d\tau\,. \tag{4.26}$$

Lemma 4.26. *For a cusp form $f \in S_k$ and $\gamma \in \mathrm{SL}_2(\mathbb{Z})$ we have*

$$(P_f \mid \gamma)(X,Y) = \int_{\gamma^{-1}(0)}^{\gamma^{-1}(i\infty)} (X - Y\tau)^{k-2} f(\tau)\, d\tau\,, \tag{4.27}$$

where $\gamma(z) = \frac{az+b}{cz+d}$ for $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ as in Section 1.3.

Proof. This is Exercise 14 i). □

In particular we see that (Exercise 14 ii))

$$\begin{aligned} (P_f \mid (1+S))(X,Y) &= \left(\int_0^{\infty i} + \int_{\infty i}^{0} \right) (X - Y\tau)^{k-2} f(\tau)\, d\tau = 0\,, \\ (P_f \mid (1+U+U^2))(X,Y) &= 0\,. \end{aligned} \tag{4.28}$$

Motivated by (4.28) we define the following subspace of V_k for even $k \geq 2$

$$W_k = \ker(1+S) \cap \ker(1+U+U^2) \subset V_k\,.$$

Let $V_k^{\pm}$ denote the ± 1-eigenspaces under the action of ϵ, i.e. V_k^{+} are the symmetric and V_k^{-} are the antisymmetric polynomials. By V^{ev} and V^{od} we denote the ± 1-eigenspaces of δ, i.e. the even and odd polynomials. With this we define the symmetric $(+)$, antisymmetric $(-)$, even (ev) and odd (od) parts of W_k for $\bullet \in \{+, -, \mathrm{ev}, \mathrm{od}\}$ by

$$W_k^{\bullet} = W_k \cap V_k^{\bullet}\,.$$

Lemma 4.27. *i) We have*

$$W_k^{+} = W_k^{od}\,, \qquad W_k^{-} = W_k^{ev}\,.$$

ii) The spaces W_k and $W_k^{\pm}$ can also be written as

$$W_k = \ker(1 - T - T')\,, \tag{4.29}$$

where $T' = -U^2 S = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$ and

$$W_k^{\pm} = \ker(1 - T \mp T\epsilon)\,.$$

Proof. This is Exercise 14 iii). □

The equation (4.29) is also called **Lewis equation**. The period polynomials of cusp forms satisfy the Lewis equation and the following theorem states, that there are no more relations. More precisely the statement of the Eichler-Shimura theorem is that we get isomorphisms of S_k to $W_k^{\pm}$ (modulo a subspace of dimension one in the even case) by sending a cusp form f to the odd P_f^+ and even part P_f^- of its period polynomial P_f.

Theorem 4.28. *(Eichler-Shimura Isomorphism) The map $p_f^{\pm} : f \mapsto P_f^{\pm}$ induces isomorphisms*

$$p_f^+ : S_k \xrightarrow{\sim} \mathbb{C} \otimes W_k^+ , \qquad p_f^- : S_k \xrightarrow{\sim} \mathbb{C} \otimes W_k^- \big/ \mathbb{Q}(X^{k-2} - Y^{k-2}) .$$

Moreover, one can show that everything is "defined over $\mathbb{Q}$", i.e. we can always find a basis of S_k, such that their images under $p_f^{\pm}$ are elements in $W_k^{\pm}$. Later we will see that we can also define period polynomials for Eisenstein series G_k, which are given exactly by a multiple of $X^{k-2} - Y^{k-2}$ in the antisymmetric (even) case. Therefore we will see that W_k^- is isomorphic to the space of all modular forms $\mathcal{M}_k$.

Example 4.29. *The odd and even parts of the period polynomial of $f = c\Delta \in S_{12}$ for some explicit $c \in \mathbb{C}$ is given by*

$$\begin{aligned} P_f^+(X,Y) &= XY(X^2-Y^2)^2(X^2-4Y^2)(4X^2-Y^2) , \\ P_f^-(X,Y) &= \frac{36}{691}(X^{10}-Y^{10}) - X^2Y^2(X^2-Y^2)^3 . \end{aligned}$$

4.3.1 The space $\mathcal{P}_k^{\mathrm{ev}}$ and its connection to $W_k^{\pm}$

Let $\mathcal{P}_k^{\mathrm{ev}} \subset \mathcal{D}_k$ denote the space spanned by all $P_{\mathrm{ev,ev}}$.

$$\begin{aligned} \mathcal{P}_k^{\mathrm{ev}} &= \langle P_{m,n} \mid m,n \geq 2 \text{ even}, m+n=k \rangle_{\mathbb{Q}} \\ &= \mathbb{Q}Z_k + \langle P_{m,n} \mid m,n \geq 4 \text{ even}, m+n=k \rangle_{\mathbb{Q}} , \end{aligned}$$

where the second equality follows from Corollary 4.11. By (4.20) we can write any $P_{m,n}$ explicitly in terms of $Z_{\mathrm{od,od}}$. In [GKZ] it was observed, that W_k^- is canonically isomorphic to $\mathcal{P}_k^{\mathrm{ev}}$, where the isomorphism can be written down explicitly by using the coefficients of period polynomials. For a $p \in W_k^-$ we define the coefficients $\beta_{k_1,k_2}^p \in \mathbb{Q}$ for $k_1, k_2 \geq 1$, $k_1 + k_2 = k$ by

$$\sum_{\substack{k_1+k_2=k \\ k_1,k_2 \geq 1}} \binom{k-2}{k_1-1} \beta_{k_1,k_2}^p X^{k_1-1} Y^{k_2-1} := p(X+Y,Y),$$

i.e. these are the coefficients of $p \mid T$ divided by $\binom{k-2}{k_1-1}$.

Theorem 4.30. *For even $k \geq 4$ the following map is an isomorphism of $\mathbb{Q}$-vector spaces*

$$\begin{aligned} W_k^- &\longrightarrow \mathcal{P}_k^{ev} \\ p &\longmapsto \sum_{\substack{k_1+k_2=k \\ k_1,k_2 \ odd}} \beta_{k_1,k_2}^p Z_{k_1,k_2} . \end{aligned}$$

Moreover the image can be written in terms of the generators of $\mathcal{P}_k^{ev}$ explicitly as

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ odd}}} \beta^p_{k_1,k_2} Z_{k_1,k_2} \equiv \frac{1}{6} \sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ even}}} \beta^p_{k_1,k_2} P_{k_1,k_2} \qquad \mod \mathbb{Q}Z_k\,.$$

Before we give a proof of this theorem, we give some application of it for our multiple zeta realization φ_ζ and our combinatorial Eisenstein realization φ_G.

Theorem 4.31. *For $k \geq 4$ the combinatorial Eisenstein realization gives an isomorphism*

$$\varphi_G : \mathcal{P}_k^{ev} \xrightarrow{\sim} \mathcal{M}_k^{\mathbb{Q}}\,.$$

Proof. By the Eichler-Shimura isomorphism (Theorem 4.28) we know that $\dim W_k^- = \dim S_k + 1 = \dim \mathcal{M}_k^{\mathbb{Q}}$, so by Theorem 4.30 it suffices to show surjectivity. By Theorem 1.19 we know that the set

$$\mathbb{Q}G_k + \langle G_m G_n \mid m,n \geq 4 \text{ even}, m+n=k\rangle_{\mathbb{Q}}$$

generates $\mathcal{M}_k^{\mathbb{Q}}$. But this is exaclty the image of the generating set of $\mathcal{P}_k^{\mathrm{ev}}$ under φ_G. □

Another consequence of Theorem 4.30 is the following.

Corollary 4.32. *Let $k \geq 4$ be even and $p \in W_k^-$.*

i) We have

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ odd}}} \beta^p_{k_1,k_2} \zeta(k_1,k_2) \in \mathbb{Q}\pi^k\,.$$

ii) We have

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ odd}}} \beta^p_{k_1,k_2} G(k_1,k_2) \in \mathcal{M}_k^{\mathbb{Q}}\,. \tag{4.30}$$

Proof. This follows from $\varphi_\zeta(\mathcal{P}_k^{\mathrm{ev}}) = \mathbb{Q}\pi^k$ and $\varphi_G(\mathcal{P}_k^{\mathrm{ev}}) = \mathcal{M}_k^{\mathbb{Q}}$ (Theorem 4.31 above). □

Remark 4.33. Starting with a cusp form $f \in S_k$ we obtain with $p = P_f$ by (4.30) a modular form and by Theorem 4.31 we get all modular forms from this. For a long time the relationship between f and this modular form was unknown. Recently it was proven by Tasaka ([Tas]) that one can get back exactly f in (4.30) by, roughly speaking, considering a slight modification of the isomorphism in Theorem 4.30.

Now we will give an analogue statement for the space W_k^+ for odd period polynomials and see that its canonically dual to $\mathcal{P}_k^{\mathrm{ev}}$:

Theorem 4.34. *For even $k \geq 4$ the following map is an isomorphism of $\mathbb{Q}$-vector spaces*

$$\begin{aligned} W_k^+ &\longrightarrow \{\varphi \in \mathrm{Hom}(\mathcal{P}_k^{ev},\mathbb{Q}) \mid \varphi(Z_k)=0\} \\ \sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 2 \text{ even}}} p_{k_1,k_2} X^{k_1-1}Y^{k_2-1} &\longmapsto (\varphi : P_{k_1,k_2} \mapsto p_{k_1,k_2})\,. \end{aligned}$$

In other words any polynomial in W_k^+ gives a realization φ of $\mathcal{P}_k^{\mathrm{ev}}$ in $\mathbb{Q}$ with $\varphi(Z_k)=0$. Later we will see that we can extend the space W_k^+ to a space from which we will actually obtain any realization of $\mathcal{P}_k^{\mathrm{ev}}$ in $\mathbb{Q}$.

To prove Theorems 4.30 and 4.34 we will use the pairing on V_k defined in (4.13) by

$$\langle X^{r-1}Y^{s-1}\,,\,X^{m-1}Y^{n-1}\rangle = \frac{(-1)^r}{\binom{k-2}{m-1}}\delta_{(r,s),(n,m)}\,.$$

Assume we have the following element in V_k

$$A(X,Y) = \sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} \binom{k-2}{k_1-1} a_{k_1,k_2} X^{k_1-1}Y^{k_2-1}\,. \tag{4.31}$$

Pairing $A\,|\,S$ with some polynomial therefore gives

$$\langle A|\,S, \sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} c_{k_1,k_2}X^{k_1-1}Y^{k_2-1}\rangle = \sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} a_{k_1,k_2}c_{k_1,k_2}\,. \tag{4.32}$$

This will be used to prove the following Lemma.

Lemma 4.35. *Let A and a_{k_1,k_2} be as in* (4.31) *and $k\geq 1$.*

i) In $\mathcal{D}_k$ the relation

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} a_{k_1,k_2}Z_{k_1,k_2} = \lambda Z_k\,,$$

holds, if and only if $A = H\,|\,(T'-1)$ for some polynomial $H\in V_k^+$. In this case we have

$$\lambda = \frac{1}{2}\langle H\,|\,\delta, \frac{X^{k-1}-Y^{k-1}}{X-Y}\rangle = \frac{k-1}{2}\int_0^1 H(t,1-t)dt\,.$$

ii) In $\mathcal{D}_k$ the relation

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} a_{k_1,k_2}P_{k_1,k_2} = \mu Z_k\,,$$

holds, if and only if $A = H\,|\,(1-S)$ for some polynomial $H\in V_k^U\cap V_k^+$. In this case we have

$$\mu = \langle H, \frac{X^{k-1}-Y^{k-1}}{X-Y}\rangle\,.$$

Here V_k^U denotes the space of U invariant polynomials, i.e. $H\,|\,U=H$.

Proof. For i) first notice that by (4.32) we have

$$\langle A|\,S, \mathfrak{Z}_k\rangle = \sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} a_{k_1,k_2}Z_{k_1,k_2}\,.$$

Now assume that $A \in V_k^+ \mid (T'-1)$. Since $V_k^+ \mid S = V_k^+$ and $T^{-1}S = ST'$ we get

$$V_k^+ \mid (T'-1) = V_k^+ \mid S(T'-1) = V_k^+ \mid (T^{-1}-1)S$$

hence $A \in V_k^+ \mid (T^{-1}-1)S$. Since $V_k^+ = V_k \mid (1+\epsilon)$ and $\Delta^* = (1+\epsilon)(T^{-1}-1)$ we obtain $A \mid S \in V_k \mid \Delta^*$ if and only if $A \in V_k^+ \mid (T'-1)$. More precisely if $A = H \mid (T'-1)$ for some $H \in V_k^+$ we therefore have by using $H = \frac{1}{2}H \mid (1+\epsilon)$ and $(1+\epsilon)S = \delta(1+\epsilon)$

$$A\,|\,S = H\,|\,(T'-1)S = H\,|\,S(T^{-1}-1) = \frac{1}{2}H\,|\,(1+\epsilon)S(T^{-1}-1) = \frac{1}{2}H\,|\,\delta(1+\epsilon)(T^{-1}-1) = \frac{1}{2}H\,|\,\delta\Delta^*\,,$$

which gives by the Γ-invariance of the pairing (Proposition 4.13) and $\mathfrak{Z}_k\,|\Delta = \mathfrak{R}_k = Z_k\frac{X^{k-1}-Y^{k-1}}{X-Y}$

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} a_{k_1,k_2} Z_{k_1,k_2} = \langle A|\,S, \mathfrak{Z}_k\rangle = \frac{1}{2}\langle H\,|\,\delta\Delta^*, \mathfrak{Z}_k\rangle = \frac{1}{2}\langle H\,|\,\delta, \mathfrak{Z}_k\,|\,\Delta\rangle = \frac{1}{2}\langle H\,|\,\delta, \mathfrak{R}_k\rangle = \lambda Z_k\,.$$

The second expression for λ follows by using the beta integral

$$\int_0^1 t^{k_1-1}(1-t)^{k_2-1}dt = \left(\binom{k-2}{k_1-1}(k-1)\right)^{-1}.$$

The proof for ii) follows by considering a symmetric version of i) together with $P_{k_1,k_2} = Z_{k_1,k_2} + Z_{k_2,k_1} + Z_k$ (Exercise 15). For this one shows that $A = H \mid (T'-1)$ for $H \in V_k^+$ is symmetric if and only if $H = H \mid U$. □

Remark 4.36. Notice that there is a 1:1 correspondence between elements $H \in V_k^+$ and the relations in Lemma 4.35 i), since $\dim V_k^+$ gives exactly the proven number of relations in $\mathcal{D}_k$, which follow from the dimension formulas in Theorem 4.6 and 4.12. In other words: For a given relation in $\mathcal{D}_k$, there exist a unique symmetric polynomial $H \in V_k^+$, which gives this relation by the construction in Lemma 4.35. This one can also prove by using that the pairing is non-degenerated, which gives another proof of the dimension formulas (without giving explicit bases).

We now have all the necessary ingredients to prove Theorem 4.30.

Proof of Theorem 4.30. First we will show that the map

$$\begin{aligned} \Theta : W_k^- &\longrightarrow \mathcal{P}_k^{\mathrm{ev}} \\ p &\longmapsto \sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ odd}}} \beta^p_{k_1,k_2} Z_{k_1,k_2} \end{aligned}$$

is well defined, i.e. that the image is actually an element in $\mathcal{P}_k^{\mathrm{ev}}$. For this we write $q = p \mid T$ and then see bv direct calculation that with $A = q^{od} - 3q^{ev}$ and $H = 2(q^{\mathrm{ev},+} - q^{\mathrm{od},+}) \in V_k^k$ (Exercise 15 i)) we have

$$A = H \mid (T'-1)\,.$$

Here one uses that p satisfies the Lewis equation and is antisymmetric to show that $q^{ev,-} = \frac{1}{2}p$ and $q^{\mathrm{od},-} = 0$. Now we can apply Lemma 4.35i) and, since the coefficients $\beta^p_{k_1,k_2}$ are (up to a binomial coefficient) defined by the coefficients of q, we obtain the relation

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ odd}}} \beta^p_{k_1,k_2} Z_{k_1,k_2} \equiv \frac{1}{3}\sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ even}}} \beta^p_{k_1,k_2} Z_{k_1,k_2} \qquad \mathrm{mod}\ \mathbb{Q}Z_k\,.$$

Further since $q^{od,-}=0$ we have $\beta^p_{k_1,k_2}=\beta^p_{k_2,k_1}$ for even $k_1,k_2\geq 2$. From this we obtain

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ odd}}} \beta^p_{k_1,k_2} Z_{k_1,k_2} \equiv \frac{1}{6} \sum_{\substack{k_1+k_2=k\\ k_1,k_2 \text{ even}}} \beta^p_{k_1,k_2} P_{k_1,k_2} \qquad \bmod \mathbb{Q}Z_k\,,$$

i.e. the map is in Θ is well-defined and the image is given as stated in the Theorem. The coefficient of Z_k can be obtained explicitly by calculating the corresponding λ in Lemma 4.35. It remains to show that Θ is bijective. We will show in the proof of Theorem 4.34 that the dimension of W_k^- and $\mathcal{P}_k^{\mathrm{ev}}$ coincide and therefore we just need to show injectivity. This follows directly since if $\theta(p)=0$, then $\beta^p_{k_1,k_2}=0$ for all $k_1,k_2\geq 1$ odd, since the $Z_{\mathrm{od},\mathrm{od}}$ are linearly independent. But then we have $p=0$ since $0=q^{ev,-}=\frac{1}{2}p$. $\square$

Using the second part of Lemma 4.35, we will now the proof of Theorem 4.34. For this, we will first show the following.

Lemma 4.37. *We have $A\in V_k^{U,+}\mid(1-S)$ if and only if $A\in V_k^{od}$ and $A\perp W_k^+$.*

Proof. Let $v\in(V_k^{U,+}\mid(1-S))^\perp$. Since $V_k^{U,+}\mid(1-S)=V_k\mid(1+U+U^2)(1+\epsilon)(1-S)$ we obtain, by using again the Γ-invariance and the fact that the pairing is non-degenerated, that

$$v\,|\,(1-S)(1+\epsilon)(1+U+U^2)=0\,.$$

But this means that

$$v\,|\,(1-S)(1+\epsilon)\in\ker(1+U+U^2)\cap\ker(1+S)\cap\ker(1-\epsilon)=W_k^+\,,$$

from which we get $v\in W_k^+ + V_k^- + V_k^{\mathrm{ev}}$. Since $V_k^{\mathrm{od}}=(V_k^{\mathrm{ev}})^\perp$ we therefore have $V_k^{U,+}\mid(1-S)=\left(W_k^+\right)^\perp\cap V_k^{\mathrm{od}}$ from which the statement follows. $\square$

Proof of Theorem 4.34. By Lemma 4.35 ii) a relation of the form

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} a_{k_1,k_2}P_{k_1,k_2}=\mu Z_k\,,$$

holds, if and only if $A\in V_k^{U,+}\mid(1-S)$. By Lemma 4.37 we therefore have that this relations holds if and only if $A\in V_k^{\mathrm{od}}$ and $A\perp W_k^+$. Since $A\mid S=A$ we therefore have $\langle A\mid S,p\rangle=0$ for any $p\in W_k^+$. If we write $p=\sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 2 \text{ even}}} p_{k_1,k_2}X^{k_1-1}Y^{k_2-1}$ we get by (4.32) that $p\in W_k^+$ if and only if

$$\sum_{\substack{k_1+k_2=k\\ k_1,k_2\geq 1}} a_{k_1,k_2}p_{k_1,k_2}=0\,.$$

And therefore the realizations $\varphi\in\mathrm{Hom}(\mathcal{P}_k^{\mathrm{ev}},\mathbb{Q})$ with $\varphi(Z_k)=0$ are exactly those given by $\varphi(P_{k_1,k_2})=p_{k_1,k_2}$ for $p\in W_k^+$. $\square$

4.3.2 Extended period polynomials

In this section we want to introduce period polynomials for all modular forms. For a modular form $f = \sum_{n\geq 0} a_n q^n \in M_k$, which is not a cusp form, i.e. $a_0 \neq 0$, the integral (4.26) does not converge. In [Za4] Zagier introduces the **extended period polynomial** for any $f = \sum_{n\geq 0} a_n q^n \in M_k$, by

$$\begin{aligned}\widehat{P}_f(X,Y) = &\int_{\tau_0}^{i\infty} (X - Y\tau)^{k-2}(f(\tau) - a_0)d\tau + \int_0^{\tau_0} (X - Y\tau)^{k-2} \left(f(\tau) - \frac{a_0}{\tau^k}\right) d\tau \\ &+ \frac{a_0}{(k-1)} \left(\frac{1}{Y} - \frac{\tau_0^{1-k}}{X}\right) (X - Y\tau_0)^{k-1} .\end{aligned} \tag{4.33}$$

Here $\tau_0 \in \mathbb{H}$ is arbitrary, and one can check that the definition of $\widehat{P}_f(X,Y)$ is independent of τ_0 since the derivative of the right-hand side with respect to τ_0 vanishes.

For example, the extended period polynomial of the Eisenstein series G_k is

$$\widehat{P}_{G_k}(X,Y) = \frac{2\pi i \zeta(k-1)}{2(k-1)}(X^{k-2} - Y^{k-2}) - \frac{(2\pi i)^k}{2(k-1)} \sum_{\substack{k_1+k_2=k \\ k_1,k_2\geq 0}} \frac{B_{k_1}}{k_1!}\frac{B_{k_2}}{k_2!} X^{k_1-1}Y^{k_2-1} .$$

In general $\widehat{P}_f(X,Y)$ is not an element in $\mathbb{C} \otimes V_k$ anymore, since we can get poles in X and Y. We therefore define the space

$$\widehat{V}_k = \bigoplus_{\substack{k_1+k_2=k \\ k_1,k_2\geq 0}} \mathbb{Q} X^{k_1-1}Y^{k_2-1} .$$

With this we have for any $f \in \mathcal{M}_k$, that $\widehat{P}_f(X,Y) \in \mathbb{C} \otimes \widehat{V}_k$. The group Γ does not act on $\widehat{V}_k$ anymore, but still it makes sense to define the following subspace of $\widehat{V}_k$

$$\widehat{W}_k := \ker(1 + U + U^2) \cap \ker(1 + S) = \ker(1 - T - T') ,$$

which contains all elements in $\widehat{V}_k$ which vanish under the actions $1 + U + U^2$ and $1 + S$ (defined in the same way as before). One can then also check, that $\widehat{P}_f(X,Y) \in \mathbb{C} \otimes \widehat{W}_k$ and we have the following extended version of the Theorem of Eichler-Shimura, where we define $\widehat{W}_k^{\pm}$ again by the symmetric and antisymmetric parts of $\widehat{W}_k$.

Theorem 4.38. *(Eichler-Shimura, Zagier [Za4]) The map $\widehat{p}_f^{\pm} : f \mapsto \widehat{P}_f^{\pm}$ induces isomorphism*

$$\widehat{p}_f^{+} : \mathcal{M}_k \xrightarrow{\sim} \mathbb{C} \otimes \widehat{W}_k^{+} , \qquad \widehat{p}_f^{-} : \mathcal{M}_k \xrightarrow{\sim} \mathbb{C} \otimes \widehat{W}_k^{-} = \mathbb{C} \otimes W_k^{-} .$$

We obtain an extended version of Theorem 4.34 given by the following.

Theorem 4.39. *For even $k \geq 4$ the following map is an isomorphism of $\mathbb{Q}$-vector spaces*

$$\begin{aligned}\widehat{W}_k^{+} &\longrightarrow \{\varphi \in \mathrm{Hom}(\mathcal{P}_k^{ev}, \mathbb{Q})\} \\ \sum_{\substack{k_1+k_2=k \\ k_1,k_2\geq 2 \ even}} p_{k_1,k_2} X^{k_1-1}Y^{k_2-1} &\longmapsto (\varphi : P_{k_1,k_2} \mapsto p_{k_1,k_2}) .\end{aligned}$$

Proof. Corresponding to the splitting $\mathcal{M}_k = S_k \oplus \mathbb{C}G_k$ we also have $\widehat{W}_k^+ = W_k^+ \oplus \mathbb{Q}\mathcal{E}_k^+$, where

$$\mathcal{E}_k = \sum_{\substack{k_1+k_2=k \\ k_1,k_2\geq 0}} \binom{k}{k_1} B_{k_1} B_{k_2} X^{k_1-1} Y^{k_2-1} \,.$$

The theorem follows then by Theorem 4.34 together with the fact that the image of $\mathcal{E}_k$ gives exactly the realization φ_β given in Theorem 4.20, which satisfies $\varphi_\beta(Z_k) \neq 0$. □

There is also a (non-unique) way to lift the realizations in 4.39 of $\mathcal{P}_k^{\mathrm{ev}}$ to realizations of $\mathcal{D}_k$ in $\mathbb{Q}$.

Theorem 4.40. *Let $\widetilde{P} = P + \lambda(X^{k-1}Y^{-1} + X^{-1}Y^{k-1}) \in \widetilde{W}_k^+$ where $P \in W_k^+$ and define*

$$Z = \frac{1}{3} P \,|\, (T^{-1} + 1) + \frac{\lambda}{6} \frac{X^{k-1} - Y^{k-1}}{X - Y} \,|\, (5 - 3U + U\epsilon).$$

Then we have

$$P = Z \,|\, (1 + \epsilon) - 2\lambda \frac{X^{k-1} - Y^{k-1}}{X - Y} = Z \,|\, T(1 + \epsilon) \,.$$

In particular we get a realization φ of $\mathcal{D}_k$ in $\mathbb{Q}$ by $\varphi(Z_k) = -2\lambda$ and

$$\begin{aligned} \varphi(Z_{k_1,k_2}) &= \text{coefficient of } X^{k_1-1}Y^{k_2-1} \text{ in } Z(X,Y)\,, \\ \varphi(P_{k_1,k_2}) &= \text{coefficient of } X^{k_1-1}Y^{k_2-1} \text{ in } P(X,Y) \end{aligned}$$

Proof. This can be checked by direct calculation. □

The realization φ_β (Theorem 4.20) can be seen as a special case of Theorem 4.40 by choosing $\widetilde{P} = \mathcal{E}_k$.

§5 Multiple Eisenstein series and q-analogues of MZV

In this section, we will introduce multiple Eisenstein series, calculate their Fourier expansion, and explain their connection to q-analogues of multiple zeta values. Multiple Eisenstein series were introduced in [GKZ] (in the depth 2 case) and then in [B0] (See also [B1])the author calculated their Fourier expansion in arbitrary depths. Later in [BT], the authors extended the definition to all indices and gave a connection to the so-called Goncharov coproduct of formal iterated integrals. In the whole section we will will always write $q = e^{2\pi i\tau}$ for $\tau \in \mathbb{H}$.

Recall that we defined in Section 1.3.1 the Eisenstein series $\mathbb{G}_k$ for $k \geq 4$ and $\tau \in \mathbb{H}$ by

$$\mathbb{G}_k(\tau) = \frac{1}{2} \sum_{\substack{m,n\in\mathbb{Z} \\ (m,n)\neq(0,0)}} \frac{1}{(m\tau+n)^k} \,. \tag{5.1}$$

Splitting the summation into the parts $m = 0$ and $m \in \mathbb{Z}\backslash 0$ we obtain for even k

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

To calculate the Fourier expansion of the sum on the right, one uses the following.

Proposition 5.1. *(Lipschitz summation formula) For $k \geq 2$ and $q = e^{2\pi i\tau}$ we have*

$$\sum_{n\in\mathbb{Z}} \frac{1}{(\tau+n)^k} = \frac{(-2\pi i)^k}{(k-1)!} \sum_{d=1}^{\infty} d^{k-1} q^d \,. \tag{5.2}$$

Proof. Consider the partial fraction expansion and Fourier expansion of the coth

$$\frac{1}{\tau} + \sum_{n=1}^{\infty} \left(\frac{1}{\tau-n} + \frac{1}{\tau+n} \right) = \pi\cot(\pi\tau) = -\pi i - 2\pi i \sum_{d=1}^{\infty} q^d \,.$$

Taking the $k-1$-th derivative on both sides yields (5.2). □

With (5.2) we obtain

$$\begin{aligned}
\mathbb{G}_k(\tau) &= \zeta(k) + \frac{(-2\pi i)^k}{(k-1)!} \sum_{m=1}^{\infty}\sum_{d=1}^{\infty} d^{k-1} q^{mn} \\
&= \zeta(k) + \frac{(-2\pi i)^k}{(k-1)!} \sum_{n=1}^{\infty} \sigma_{k-1}(n) q^n \\
&= \zeta(k) + (-2\pi i)^k \, \mathrm{g}(k) \,,
\end{aligned} \tag{5.3}$$

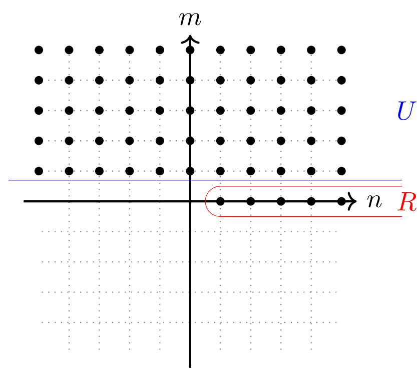
Here and in the following we will always surpress the dependence of $\mathrm{g}(k)$ on τ and always view it as a function in τ with $q = e^{2\pi i\tau}$. Formula (5.3) also makes sense for odd k but does not give a modular form, since there are no non trivial modular forms of odd weight. In the following, we want to construct a "multiple version" of $\mathbb{G}_k$, such that its constant term gives multiple zeta values.
The sum in (5.1) 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 a multiple version of the Eisenstein series in an obvious way.

Definition 5.2. *Let $\tau \in \mathbb{H}$. We define the order $\succ$ on $\mathbb{Z}\tau + \mathbb{Z}$ for $\lambda_1, \lambda_2 \in \mathbb{Z}\tau + \mathbb{Z}$ by*

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

where P, the **set of positive lattice points**, *is defined by*

$$P := \{m\tau + n \in \mathbb{Z}\tau + \mathbb{Z} \mid m > 0 \vee (m = 0 \wedge n > 0)\} = U \cup R\,.$$



The set P for the case $\tau = i$.

In other words we have $m_1\tau + n_1 \succ m_2\tau + n_2$ if $m_1 > m_2$ or if $m_1 = m_2$ and $n_1 > n_2$.

Since $P \cup (-P) = \Lambda_\tau \backslash \{0\}$ the Eisenstein series can be written for even $k \geq 4$ as

$$\mathbb{G}_k(\tau) = \frac{1}{2} \sum_{\substack{m,n \in \mathbb{Z} \\ (m,n) \neq (0,0)}} \frac{1}{(m\tau + n)^k} = \sum_{\substack{\lambda \succ 0 \\ \lambda \in \Lambda_\tau}} \frac{1}{\lambda^k}\,. \qquad (k \geq 4 \text{ even})$$

But now the right-hand side does not vanish anymore for odd k and we can use it to define for $\mathbb{G}_k$ all $k \geq 3$ (Since the sum converges absolutely for $k > 2$). With the same argument as before we obtain

$$\mathbb{G}_k(\tau) := \sum_{\substack{\lambda \succ 0 \\ \lambda \in \Lambda_\tau}} \frac{1}{\lambda^k} = \zeta(k) + (-2\pi i)^k\, \mathrm{g}(k)\,. \qquad (k \geq 3)$$

In general we will define the multiple version of these objects as follows.

Definition 5.3. *For $k_1 \geq 3, k_2, \dots, k_r \geq 2$ the* **multiple Eisenstein series** *are defined by*

$$\mathbb{G}_{k_1,\dots,k_r}(\tau) := \sum_{\substack{\lambda_1 \succ \dots \succ \lambda_r \succ 0 \\ \lambda_i \in \mathbb{Z}\tau + \mathbb{Z}}} \frac{1}{\lambda_1^{k_1} \dots \lambda_r^{k_r}}\,. \tag{5.4}$$

By $k = k_1 + \dots + k_r$ we denote its weight and by r its depth.

That the sum (5.4) converges absolutely for $k_1 \geq 3, k_2, \dots, k_r \geq 2$ can be checked by generalizing the proofs of Theorems 4.3 and B.1 in [C]. The multiple Eisenstein series are holomorphic functions in the upper half-plane and they satisfy the stuffle product formula, i.e. for example we have

$$\mathbb{G}_3(\tau) \cdot \mathbb{G}_4(\tau) = \mathbb{G}_{4,3}(\tau) + \mathbb{G}_{3,4}(\tau) + \mathbb{G}_7(\tau)\,.$$

But, as we already see in depth one, they are in general not modular forms. The Eisenstein series $\mathbb{G}_2$ does not converge absolulеltey but is conditionally convergent. We define it by

$$\mathbb{G}_2(k) := \lim_{M\to\infty} \lim_{N\to\infty} \sum_{M>m>0} \sum_{-N<n<N} \frac{1}{(m\tau+n)^2} = \zeta(2) + \widehat{\mathrm{g}}(2)$$

i.e. we sum first "horizontally" the n and then "vertically" the m. This is usually called **Eisenstein summation**. In general set $\mathbb{Z}_M = \{m \in \mathbb{Z} \mid |m| < M\}$ for an integer $M > 0$. With this we define the multiple Eisenstein series for all $k_1, \ldots, k_r \geq 2$ by

$$\mathbb{G}_{k_1,\ldots,k_r}(\tau) := \lim_{M\to\infty} \lim_{N\to\infty} \sum_{\substack{\lambda_1 \succ \cdots \succ \lambda_r \succ 0 \\ \lambda_i \in \mathbb{Z}_M\tau + \mathbb{Z}_N}} \frac{1}{\lambda_1^{k_1} \ldots \lambda_r^{k_r}} . \tag{5.5}$$

These also satisfy for all $k_1, \ldots, k_r \geq 2$ the stuffle product formula, since one can check easily that this is already true for fixed M and N.

5.1 The Fourier expansion of multiple Eisenstein series

By definition it is $\mathbb{G}_{k_1,\ldots,k_r}(\tau+1) = \mathbb{G}_{k_1,\ldots,k_r}(\tau)$, i.e. there exists a Fourier expansion of $\mathbb{G}_{k_1,\ldots,k_r}$. In depth one we already saw that this is the case:

$$\mathbb{G}_k(\tau) = \zeta(k) + (-2\pi i)^k \,\mathrm{g}(k) .$$

We will see that it will be possible in general to write $\mathbb{G}_{k_1,\ldots,k_r}$ in terms of multiple zeta values and $(-2\pi i)^{k_1+\cdots+k_r} \,\mathrm{g}(k_1, \ldots, k_r)$. Therefore we define for all $k_1, \ldots, k_r \geq 1$

$$\widehat{\mathrm{g}}(k_1, \ldots, k_r) := (-2\pi i)^{k_1+\cdots+k_r} \,\mathrm{g}(k_1, \ldots, k_r) \tag{5.6}$$

which then gives $\mathbb{G}_k(\tau) = \zeta(k)+\widehat{\mathrm{g}}(k)$. Again in everything that follows $\widehat{\mathrm{g}}$ can be viewed as a holomorphic function in τ but we will avoid to write $\widehat{\mathrm{g}}(k_1, \ldots, k_r; \tau)$ in order to make notations shorter.

Theorem 5.4. *The $\mathbb{G}_{k_1,\ldots,k_r}(\tau)$ can be written as a $\mathcal{Z}$-linear combination of $\widehat{\mathrm{g}}$.*
More precisely, for $k_1, \ldots, k_r \geq 2$ there exist rational numbers $\alpha_j^{(l_1,\ldots,l_r)} \in \mathbb{Q}$, for $l_1, \ldots, l_r \geq 2$ and $1 \leq j \leq r-1$ with $k = k_1 + \cdots + k_r = l_1 + \cdots + l_r$, such that

$$\mathbb{G}_{k_1,\ldots,k_r}(\tau) \;=\; \zeta(k_1, \ldots, k_r) \;+ \sum_{\substack{1\leq j\leq r-1 \\ l_1,\ldots,l_r \geq 2 \\ l_1+\cdots+l_r=k}} \alpha_j^{(l_1,\ldots,l_r)} \cdot \zeta(l_1, \ldots, l_j) \cdot \widehat{\mathrm{g}}(l_{j+1}, \ldots, l_r) \;+\; \widehat{\mathrm{g}}(k_1, \ldots, k_r) .$$

The rest of this section will be devoted to prove this Theorem. For example, the triple Eisenstein series $\mathbb{G}_{3,2,2}$ can be written as

$$\begin{aligned}\mathbb{G}_{3,2,2}(\tau) =& \zeta(3,2,2) + \left(\frac{54}{5}\zeta(2,3) + \frac{51}{5}\zeta(3,2)\right)\widehat{\mathrm{g}}(2) + \frac{16}{3}\zeta(2,2)\widehat{\mathrm{g}}(3) \\ &+ 3\zeta(3)\widehat{\mathrm{g}}(2,2) + 4\zeta(2)\widehat{\mathrm{g}}(3,2) + \widehat{\mathrm{g}}(3,2,2) .\end{aligned}$$

To derive the Fourier expansion, we introduce the following functions, which 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 5.5. *For $k_1, \dots, k_r \geq 2$ and $x \in \mathbb{C}\backslash\mathbb{Z}$ we define the multitangent function of depth r by*

$$\Psi_{k_1,\dots,k_r}(x) = \sum_{\substack{n_1 > \cdots > n_r \\ n_i \in \mathbb{Z}}} \frac{1}{(x+n_1)^{k_1} \dots (x+n_r)^{k_r}} \,.$$

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

These functions were introduced and studied in detail by Bouillot in [Bo]. One of the main results in [Bo], 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 5.6. *([Bo, Theorem 3], Reduction of multitangent into monotangent functions) For $k_1, \dots, k_r \geq 2$ and $k = k_1 + \cdots + k_r$ the multitangent function can be written as a $\mathcal{Z}$-linear combination of monotangent functions, more precisely there are $c_j^{k_1,\dots,k_r} \in \mathcal{Z}_{k-j}$ such that*

$$\Psi_{k_1,\dots,k_r}(x) = \sum_{j=2}^{k} c_j^{k_1,\dots,k_r} \Psi_j(x) \,.$$

Proof. An explicit formula for the coefficients $c_j^{k_1,\dots,k_r}$ is given in Theorem 3 in [Bo] . The proof uses partial fraction and a non trivial relation between multiple zeta values (see [BT] Lemma 2.4) to argue that the sum starts at $j = 2$. For example in length two it is

$$\begin{aligned} \Psi_{3,2}(x) &= \sum_{n_1 > n_2} \frac{1}{(x+n_1)^3 (x+n_2)^2} \\ &= \sum_{n_1>n_2} \left(\frac{1}{(n_1-n_2)^2 (x+n_1)^3} + \frac{2}{(n_1-n_2)^3 (x+n_1)^2} + \frac{3}{(n_1-n_2)^4 (x+n_1)} \right) \\ &+ \sum_{n_1>n_2} \left(\frac{1}{(n_1-n_2)^3 (x+n_2)^2} - \frac{3}{(n_1-n_2)^4 (x+n_2)} \right) \\ &= 3\zeta(3)\Psi_2(x) + \zeta(2)\Psi_3(x) \,. \end{aligned} \tag{5.7}$$

□

The connection between the functions $\widehat{\mathrm{g}}$ and the monotangent functions is given by the following

Proposition 5.7. *For $k_1, \dots, k_r \geq 2$ the functions $\widehat{\mathrm{g}}$ can be written as*

$$\widehat{\mathrm{g}}(k_1, \dots, k_r) = \sum_{m_1 > \cdots > m_r > 0} \Psi_{k_1}(m_1\tau) \dots \Psi_{k_r}(m_r\tau) \,.$$

Proof. This follows directly from the Lipschitz formula (5.2) and the definition of the functions $\widehat{\mathrm{g}}$, since

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

and therefore

$$\begin{aligned} \sum_{m_1 > \cdots > m_r > 0} \Psi_{k_1}(m_1\tau) \dots \Psi_{k_r}(m_r\tau) &= (-2\pi i)^{k_1+\cdots+k_r} \sum_{\substack{m_1 > \cdots > m_r > 0 \\ d_1,\dots,d_r > 0}} \frac{d^{k_1-1}}{(k_1-1)!} \cdots \frac{d^{k_r-1}}{(k_r-1)!} q^{m_1 d_1 + \cdots + m_r d_r} \\ &= (-2\pi i)^{k_1+\cdots+k_r} \, \mathrm{g}(k_1, \dots, k_r) = \widehat{\mathrm{g}}(k_1, \dots, k_r) \,. \end{aligned}$$

□

Preparation for the Proof of Theorem 5.4: We will now recall the construction of the Fourier expansion of multiple Eisenstein series introduced in [B0], in order to prove Theorem 5.4. To calculate the Fourier expansion we rewrite the multiple Eisenstein series as

$$\mathbb{G}_{k_1,\dots,k_r}(\tau) = \sum_{\lambda_1 \succ \dots \succ \lambda_r \succ 0} \frac{1}{\lambda_1^{k_1} \dots \lambda_r^{k_r}}$$
$$= \sum_{(\lambda_1,\dots,\lambda_r) \in P^r} \frac{1}{(\lambda_1 + \dots + \lambda_r)^{k_1} (\lambda_2 + \dots + \lambda_r)^{k_2} \dots \lambda_r^{k_r}} .$$

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

$$\mathbb{G}^{A_1 \dots A_r}_{k_1,\dots,k_r}(\tau) := \sum_{(\lambda_1,\dots,\lambda_r) \in A_1 \times \dots \times A_r} \frac{1}{(\lambda_1 + \dots + \lambda_r)^{k_1} (\lambda_2 + \dots + \lambda_r)^{k_2} \dots \lambda_r^{k_r}}$$

this gives the decomposition

$$\mathbb{G}_{k_1,\dots,k_r} = \sum_{A_1,\dots,A_r \in \{R,U\}} \mathbb{G}^{A_1 \dots A_r}_{k_1,\dots,k_r} .$$

In the following, we identify the $A_1 \dots A_r$ with words in the alphabet $\{R, U\}$. We first illustrate the general algorithm in depth one and two.

Example 5.8. *i) In depth $r = 1$ we have $\mathbb{G}_k(\tau) = \mathbb{G}^R_k(\tau) + \mathbb{G}^U_k(\tau)$ and*

$$\mathbb{G}^R_k(\tau) = \sum_{\substack{m_1=0 \\ n_1>0}} \frac{1}{(0\tau + n_1)^k} = \zeta(k) ,$$
$$\mathbb{G}^U_k(\tau) = \sum_{\substack{m_1>0 \\ n_1 \in \mathbb{Z}}} \frac{1}{(m_1\tau + n_1)^k} = \sum_{m_1>0} \Psi_k(m_1\tau) = \widehat{\mathrm{g}}(k) ,$$

which gives $\mathbb{G}_k(\tau) = \zeta(k) + \widehat{\mathrm{g}}(k)$.

ii) In depth 2 we have $\mathbb{G}_{k_1,k_2} = \mathbb{G}^{RR}_{k_1,k_2} + \mathbb{G}^{UR}_{k_1,k_2} + \mathbb{G}^{RU}_{k_1,k_2} + \mathbb{G}^{UU}_{k_1,k_2}$. The RR and UU part is similar to the depth one case and we get

$$\mathbb{G}^{RR}_{k_1,k_2} = \sum_{\substack{m_1=m_2=0 \\ n_1>n_2>0}} \frac{1}{(0\tau + n_1)^{k_1}(0\tau + n_2)^{k_r}} = \zeta(k_1, k_2) ,$$
$$\mathbb{G}^{UU}_{k_1,k_2} = \sum_{\substack{m_1>m_2>0 \\ n_1,n_2 \in \mathbb{Z}}} \frac{1}{(m_1\tau + n_1)^{k_1}(m_2\tau + n_2)^{k_r}} = \sum_{m_1>m_2>0} \Psi_{k_1}(m_1\tau)\Psi_{k_2}(m_2\tau) = \widehat{\mathrm{g}}(k_1, k_2) .$$

For the word UR we get

$$\mathbb{G}^{UR}_{k_1,k_2} = \sum_{\substack{m_1>0, m_2=0 \\ n_1 \in \mathbb{Z}, n_2>0}} \frac{1}{(m_1\tau + n_1)^{k_1}(0\tau + n_2)^{k_1}} = \sum_{m_1>0} \Psi_{k_1}(m_1\tau) \sum_{n_2>0} \frac{1}{n_2^{k_2}} = \widehat{\mathrm{g}}(k_1)\zeta(k_2) .$$

Finally, to evaluate the RU part, we need to use Theorem 5.6 which gives

$$\Psi_{k_1,k_2}(x) = \sum_{j=2}^{k_1+k_2} c_j^{k_1,k_2} \Psi_j(x) .$$

Using this we can write

$$\begin{aligned}
\mathbb{G}^{RU}_{k_1,k_2}(\tau) &= \sum_{\substack{m_1=0, m_2>0\\ n_1>n_2\\ n_i\in\mathbb{Z}}} \frac{1}{(m_1\tau+n_1)^{k_1}(m_1\tau+n_2)^{k_2}} = \sum_{m>0} \Psi_{k_1,k_2}(m\tau) = \sum_{j=2}^{k} c_j^{k_1,k_2} \sum_{m>0} \Psi_j(m\tau)\\
&= \sum_{j=2}^{k_1+k_2} c_j^{k_1,k_2}\, \widehat{\mathrm{g}}(j) .
\end{aligned}$$

In total we therefore obtain

$$\mathbb{G}_{k_1,k_2}(\tau) = \zeta(k_1,k_2) + \zeta(k_2)\widehat{\mathrm{g}}(k_1) + \sum_{j=2}^{k_1+k_2} c_j^{k_1,k_2}\, \widehat{\mathrm{g}}(j) + \widehat{\mathrm{g}}(k_1,k_2)$$

with $c_j^{k_1,k_2} \in \mathcal{Z}_{k_1+k_2-j}$.

In general, by using Proposition 5.7 the $\mathbb{G}^{U^r}_{k_1,\dots,k_r}$ can be written as

$$\begin{aligned}
\mathbb{G}^{U^r}_{k_1,\dots,k_r}(\tau) &= \sum_{\substack{m_1>\dots>m_r>0\\ n_1,\dots,n_r\in\mathbb{Z}}} \frac{1}{(m_1\tau+n_1)^{k_1}\dots(m_r\tau+n_r)^{k_r}}\\
&= \sum_{m_1>\dots>m_r>0} \Psi_{k_1}(m_1\tau)\dots\Psi_{k_r}(m_r\tau) = \widehat{\mathrm{g}}(k_1,\dots,k_r) .
\end{aligned}$$

The other special case $\mathbb{G}^{R^r}_{k_1,\dots,k_r}$ can also be written down explicitly:

$$\mathbb{G}^{R^r}_{k_1,\dots,k_r}(\tau) = \sum_{\substack{m_1=\dots=m_r=0\\ n_1>\dots>n_r>0}} \frac{1}{(0\tau+n_1)^{k_1}\dots(0\tau+n_r)^{k_r}} = \zeta(k_1,\dots,k_r) .$$

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

$$\mathbb{G}^{w}_{k_1,\dots,k_r}(\tau) = \mathbb{G}^{w'}_{k_1,\dots,k_{r-l}}(\tau)\cdot\zeta(k_{r-l+1},\dots,k_r) .$$

For example we have $\mathbb{G}^{RUURR}_{3,4,5,6,7} = \mathbb{G}^{RUU}_{3,4,5}\cdot\zeta(6,7)$. 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 $r_1,\dots,r_j \ge 1$ with $w = R^{r_1-1}UR^{r_2-1}U\dots R^{r_j-1}U$. With this one can write

$$\mathbb{G}^{w}_{k_1,\dots,k_r}(\tau) = \sum_{m_1>\dots>m_j>0} \Psi_{k_1,\dots,k_{r_1}}(m_1\tau)\cdot\Psi_{k_{r_1+1},\dots,k_{r_1+r_2}}(m_2\tau)\dots\Psi_{k_{r-r_j+1},\dots,k_r}(m_j\tau) ,$$

which give a $\mathcal{Z}$-linear combination of $\widehat{\mathrm{g}}$ by using Theorem 5.6.

Example 5.9. *For example for the word $w = RURRU$ then we have*

$$\begin{aligned}
\mathbb{G}^{RURRU}_{k_1,\dots,k_5}(\tau) &= \sum_{m_1>m_2>0} \Psi_{k_1,k_2}(m_1\tau)\Psi_{k_3,k_4,k_5}(m_2\tau) \\
&= \sum_{m_1>m_2>0} \sum_{\substack{2\le j_1\le k_1+k_2 \\ 2\le j_2\le k_3+k_4+k_5}} c^{k_1,k_2}_{j_1} c^{k_3,k_4,k_5}_{j_2} \Psi_{j_1}(m_1\tau)\Psi_{j_2}(m_2\tau) \\
&= \sum_{\substack{2\le j_1\le k_1+k_2 \\ 2\le j_2\le k_3+k_4+k_5}} c^{k_1,k_2}_{j_1} c^{k_3,k_4,k_5}_{j_2} \,\widehat{\mathrm{g}}(j_1,j_2)\,.
\end{aligned}$$

See Figure 3 for an example of a summand of $\mathbb{G}^{RURRU}_{k_1,\dots,k_5}(\tau)$.

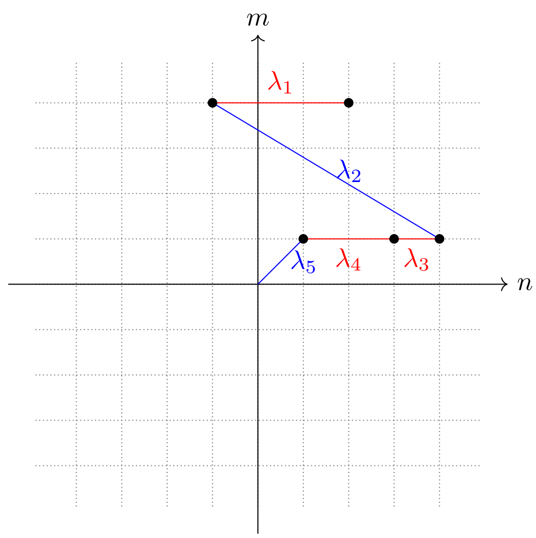


Figure 3: A summand of $\mathbb{G}^{RURRU}_{k_1,\dots,k_5}(\tau)$ for $\tau = i$.

Proof of Theorem 5.4: For $k_1,\dots,k_r \ge 2$ the Fourier expansion of the multiple Eisenstein series $\mathbb{G}_{k_1,\dots,k_r}$ can be computed in the following way

i) Split up the summation into 2^r distinct parts $\mathbb{G}^{w}_{k_1,\dots,k_r}$ where w are a words in $\{R,U\}$.

ii) For w being a word ending in R one can write $\mathbb{G}^{w}_{k_1,\dots,k_r}$ as $\mathbb{G}^{w'}_{k_1,\dots} \cdot \zeta(\dots,k_r)$ with w' ending in U.

iii) For $w = R^{r_1-1}UR^{r_2-1}U\dots R^{r_j-1}U$ being a word ending in U one can write $\mathbb{G}^{w}_{k_1,\dots,k_r}$ as

$$\mathbb{G}^{w}_{k_1,\dots,k_r}(\tau) = \sum_{m_1>\dots>m_j>0} \Psi_{k_1,\dots,k_{r_1}}(m_1\tau)\cdot\Psi_{k_{r_1+1},\dots,k_{r_1+r_2}}(m_2\tau)\dots\Psi_{k_{r-r_j+1},\dots,k_r}(m_j\tau)\,.$$

iv) Using the Theorem 5.6 we can write the multitangent functions in iii) as a $\mathcal{Z}$-linear combination of monotangents. We therefore just have $\mathcal{Z}$-linear combinations with sums of the form

$$\sum_{m_1>\dots>m_j>0} \Psi_{k_1}(m_1\tau)\dots\Psi_{k_j}(m_j\tau) = \widehat{\mathrm{g}}(k_1,\dots,k_j)\,.$$

□

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

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

Proposition 5.10. *i) ([GKZ, Formula (52)], [B0], [BT]) For $k_1, k_2 \geq 2$ the Fourier expansion of the double Eisenstein series is given by*

$$\mathbb{G}_{k_1,k_2}(\tau) = \zeta(k_1,k_2) + \zeta(k_2)\widehat{\mathrm{g}}(k_1) + \sum_{\substack{l_1+l_2=k_1+k_2\\ l_1,l_2\geq 2}} C^{l_2}_{k_1,k_2}\zeta(l_2)\widehat{\mathrm{g}}(l_1) + \widehat{\mathrm{g}}(k_1,k_2).$$

ii) ([B0], [BT]) For $k_1, k_2, k_3 \geq 2$ and $k = k_1 + k_2 + k_3$ the Fourier expansion of the triple Eisenstein series can be written as

$$\begin{aligned}
\mathbb{G}_{k_1,k_2,k_3}(\tau) &= \zeta(k_1,k_2,k_3) + \zeta(k_2,k_3)\widehat{\mathrm{g}}(k_1) + \zeta(k_3)\widehat{\mathrm{g}}(k_1,k_2) + \widehat{\mathrm{g}}(k_1,k_2,k_3)\\
&+ \zeta(k_3)\sum_{l_1+l_2=k_1+k_2} C^{l_1}_{k_1,k_2}\zeta(l_1)\widehat{\mathrm{g}}(l_2)\\
&+ \sum_{l_1+l_2=k_1+k_2} C^{l_2}_{k_1,k_2}\zeta(l_2)\widehat{\mathrm{g}}(l_1,k_3) + \sum_{l_1+l_2=k_2+k_3} C^{l_2}_{k_2,k_3}\zeta(l_2)\widehat{\mathrm{g}}(k_1,l_1)\\
&+ \sum_{l_1+l_2+l_3=k} (-1)^{k_2+k_3}\binom{l_2-1}{k_2-1}\binom{l_3-1}{k_3-1}\zeta(l_3,l_2)\widehat{\mathrm{g}}(l_1)\\
&+ \sum_{l_1+l_2+l_3=k} (-1)^{k_1+k_2+l_2+l_3}\binom{l_2-1}{l_3-1}\binom{l_3-1}{k_2-1}\zeta(l_3,l_2)\widehat{\mathrm{g}}(l_1)\\
&+ (-1)^{k_1+k_3}\sum_{l_1+l_2+l_3=k} (-1)^{l_2}\binom{l_2-1}{k_1-1}\binom{l_3-1}{k_3-1}\zeta(l_3)\zeta(l_2)\widehat{\mathrm{g}}(l_1),
\end{aligned}$$

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

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 $\mathbb{G}_2\cdot\mathbb{G}_3 = \mathbb{G}_{2,3}+\mathbb{G}_{3,2}+\mathbb{G}_5$. On the other hand we have

$$\mathbb{G}_2(\tau)\cdot\mathbb{G}_3(\tau) = (\zeta(2)+\widehat{\mathrm{g}}(2))(\zeta(3)+\widehat{\mathrm{g}}(3)) = \zeta(2)\zeta(3) + \zeta(3)\widehat{\mathrm{g}}(2) + \zeta(2)\widehat{\mathrm{g}}(3) + \widehat{\mathrm{g}}(2)\cdot\widehat{\mathrm{g}}(3).$$

and by Proposition 5.10 we obtain

$$\begin{aligned}
\mathbb{G}_{2,3}(\tau) &= \zeta(2,3) - 2\zeta(3)\widehat{\mathrm{g}}(2) + \zeta(2)\widehat{\mathrm{g}}(3) + \widehat{\mathrm{g}}(2,3),\\
\mathbb{G}_{3,2}(\tau) &= \zeta(3,2) + 3\zeta(3)\widehat{\mathrm{g}}(2) + \zeta(2)\widehat{\mathrm{g}}(3) + \widehat{\mathrm{g}}(3,2).
\end{aligned}$$

In conclusion, we obtain $\widehat{\mathrm{g}}(2)\cdot\widehat{\mathrm{g}}(3) = \widehat{\mathrm{g}}(3,2) + \widehat{\mathrm{g}}(2,3) + \widehat{\mathrm{g}}(5) + 2\zeta(2)\widehat{\mathrm{g}}(3)$. Dividing out $(-2\pi i)^5$ gives

$$\mathrm{g}(2)\cdot\mathrm{g}(3) = \mathrm{g}(3,2) + \mathrm{g}(2,3) + \mathrm{g}(5) - \frac{1}{12}\,\mathrm{g}(3),$$

which we already saw in (1.24) as a special case of Proposition 1.29.

5.2 Regularized multiple Eisenstein series

The multiple Eisenstein series $\mathbb{G}_{k_1,\dots,k_r}$ were just defined for $k_1,\dots,k_r \geq 2$ in the previous section and we saw that they have a Fourier expansion of the form

$$\mathbb{G}_{k_1,\dots,k_r}(\tau) = \zeta(k_1,\dots,k_r) + \sum_{n=1}^{\infty} a_n q^n \,. \qquad (a_n \in \mathcal{Z}[\pi i] = \mathcal{Z} + \pi i \mathcal{Z}) \tag{5.8}$$

A natural question therefore is, if there exist a "good" extension of these objects for all admissible indices $k_1 \geq 2, k_2, \dots, k_r \geq 1$. By "good" one could have different properties in mind that should be satisfied by these extended objects. One certainly is that they also should have a Fourier expansion of the form (5.8). Another property could be that the extended version also satisfies the shuffle or stuffle product formula. We want to present two types of regularization: The shuffle regularized multiple Eisenstein series ([BT]), and stuffle regularized multiple Eisenstein series ([B4]). 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 and a coproduct on $\mathfrak{H}^1_*$ together with a result on regularization of multitangent functions by O. Bouillot ([Bo]).
First recall from last section, that for $k_1,\dots,k_r \geq 2$ the $\mathbb{G}_{k_1,\dots,k_r}$ satisfy the stuffle product formula. We define $\mathbb{Q}$-vector space $\mathfrak{H}^2 = \mathbb{Q}\langle z_2, z_3, \dots\rangle \subset \mathfrak{H}^1$. Equipped with the stuffle product $*$, one can see easily that we obtain a subalgebra $\mathfrak{H}^2_* \subset \mathfrak{H}^1_*$. Now we can view the multiple Eisenstein series as an algebra homomorphism defined on the generators by

$$\begin{aligned} \mathbb{G} : \mathfrak{H}^2_* &\longrightarrow \mathcal{Z}[\pi \mathrm{i}][\![\mathrm{q}]\!] \\ z_{k_1}\cdots z_{k_r} &\longmapsto \mathbb{G}_{k_1,\dots,k_r} \,. \end{aligned}$$

By abuse of notation we will use $\mathbb{G}$ for both the map and the multiple Eisenstein series. The rough idea to extend the map $\mathbb{G}$ to $\mathfrak{H}^1$ will be as follows. On the algebra $\mathfrak{H}^1_{\sqcup\!\sqcup}$ one can define the Goncharov coproduct Δ_G and on $\mathfrak{H}^1_*$ one can define the deconcatenation coproduct Δ_H. In addition to this we will construct algebra homomorphisms ($\bullet \in \{*, \sqcup\!\sqcup\}$)

$$\hat{\mathrm{g}}^\bullet : \mathfrak{H}^1_\bullet \to \mathbb{Q}[2\pi i][[q]] \,.$$

With this we then can define two algebra homomorphisms $\mathbb{G}^\bullet : \mathfrak{H}^1_\bullet \to \mathbb{Q}[[q]]$ as follows[8].

$$\begin{tikzcd} \mathfrak{H}^1_{\sqcup\!\sqcup} \arrow[r, "\Delta_G"] \arrow[d, "\mathbb{G}^{\sqcup\!\sqcup}"'] & \mathfrak{H}^1_{\sqcup\!\sqcup} \otimes \mathfrak{H}^1_{\sqcup\!\sqcup} \arrow[d, "\hat{\mathrm{g}}^{\sqcup\!\sqcup}\otimes\zeta^{\sqcup\!\sqcup}"] \\ \mathcal{Z}[\pi i][\![q]\!] & \mathbb{Q}[2\pi i][\![q]\!] \otimes \mathcal{Z} \arrow[l, "m"] \end{tikzcd} \qquad \begin{tikzcd} \mathfrak{H}^1_{*} \arrow[r, "\Delta_H"] \arrow[d, "\mathbb{G}^{*}"'] & \mathfrak{H}^1_{*} \otimes \mathfrak{H}^1_{*} \arrow[d, "\hat{\mathrm{g}}^{*}\otimes\zeta^{*}"] \\ \mathcal{Z}[\pi i][\![q]\!] & \mathbb{Q}[2\pi i][\![q]\!] \otimes \mathcal{Z} \arrow[l, "m"] \end{tikzcd},$$

where in both cases m denotes the usual multiplication. These are both extension of the origional multiple Eisesntein series, in the sense that we have they following

$$\mathbb{G} = \mathbb{G}^{\sqcup\!\sqcup}|_{\mathfrak{H}^2} = \mathbb{G}^*|_{\mathfrak{H}^2} \,. \tag{5.9}$$

We start by reviewing the definition of formal iterated integrals and the coproduct defined by Goncharov. In an explicit example in depth two, we will see the connection of this coproduct and the

[8]The $\mathbb{G}^*(w)$ will depend on an integer M, for which we can take the limit $M \to \infty$ in the case when $w \in \mathfrak{H}^0$.

calculation of the Fourier expansion of multiple Eisenstein series from the previous section. This will give an indication of why (5.9) holds. After this, we give the definition of shuffle and stuffle regularized multiple Eisenstein series as presented in [BT] and [B4]. At the end of this section, we compare these two regularizations with the help of a few examples.

5.2.1 Formal iterated integrals

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

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

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 $\sqcup\!\sqcup$

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

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

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

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

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

v) The path inversion formula holds:

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

Definition 5.11. *(Goncharov coproduct) Define the coproduct Δ_G on $\mathcal{I}$ by*

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

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

Proposition 5.12. *([G, Prop. 2.2]) The triple $(\mathcal{I}, \sqcup\!\sqcup, \Delta_G)$ is a commutative graded Hopf algebra.*

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

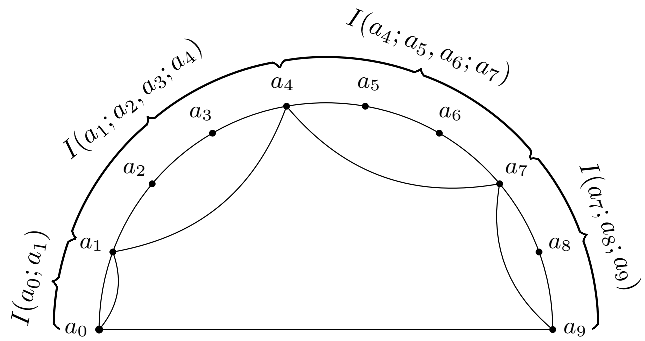


Figure 4: One diagram for the calculation of $\Delta_G\left(\mathbb{I}(a_0;a_1,\dots,a_8;a_9)\right)$. It gives the term $I(a_0;a_1,a_4,a_7;a_9)\otimes I(a_0;a_1)I(a_1;a_2,a_3;a_4)I(a_4;a_5,a_6;a_7)I(a_7;a_8;a_9)$.

For our purpose it will be important to consider the quotient space[9]

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

Let us denote by

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

the image of $\mathbb{I}(a_0;a_1,\dots,a_N;a_{N+1})$ in $\mathcal{I}^1$. The quotient map $\mathcal{I}\to\mathcal{I}^1$ 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 $\Delta_G(w_1\ \sqcup\!\sqcup\ w_2)=\Delta_G(w_1)\ \sqcup\!\sqcup\ \Delta_G(w_2)$. The coproduct on $\mathcal{I}^1$ is given by the same formula as before by replacing $\mathbb{I}$ with I. For integers $n\geq 0, k_1,\dots,k_r\geq 1$, we set

$$I_n(k_1,\dots,k_r):=I(1;\underbrace{0,0,\dots,1}_{k_1},\dots,\underbrace{0,0,\dots,1}_{k_r},\underbrace{0,\dots,0}_{n};0).$$

In particular, we write[10] $I(k_1,\dots,k_r)$ to denote $I_0(k_1,\dots,k_r)$.

Proposition 5.13. *([BT, Eq. (3.5),(3.6) and Prop. 3.5])*

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

ii) For integers $n\geq 0, k_1,\dots,k_r\geq 1$,

$$I_n(k_1,\dots,k_r)=(-1)^n\sum^{*}\left(\prod_{j=1}^{r}\binom{l_j-1}{k_j-1}\right)I(l_1,\dots,l_r)\,,$$

where the sum runs over all $l_1+\dots+l_r=k_1+\dots+k_r+n$ with $k_1,\dots,k_r\geq 1$.

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

[10] This 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).

iii) The set $\{I(k_1,\dots,k_r) \mid r \geq 0, k_i \geq 1\}$ forms a basis of the space $\mathcal{I}^1$.

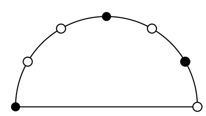
We give an example for ii): In $\mathcal{I}^1$ it is $I(1;0;0)=0$ and therefore

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

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

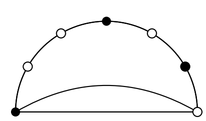
Remark 5.14. Statement iii) in Proposition 5.13 basically states that we can identify $\mathcal{I}^1$ with $\mathfrak{H}^1$ by sending $I(k_1,\dots,k_r)$ to $z_{k_1}\dots z_{k_r}$, which is an algebra isomorphism with respect to the shuffle product. In other words, we can equip $\mathfrak{H}^1$ with the coproduct Δ_G. Instead of working with I we will use this identification in the next section when defining the shuffle regularized multiple Eisenstein series.

Example 5.15. *In the following we are going to calculate $\Delta_G(I(3,2)) = \Delta_G(I(1;0,0,1,0,1;0))$. 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 $\mathbb{G}_{3,2}(\tau)$ using the construction described in Section 5. Recall that we also had the 4 different parts $\mathbb{G}^{RR}_{3,2}$, $\mathbb{G}^{UR}_{3,2}$, $\mathbb{G}^{RU}_{3,2}$ and $\mathbb{G}^{UU}_{3,2}$. 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 $\mathbb{G}^w$.

i) Diagrams with no marked $\bullet$:

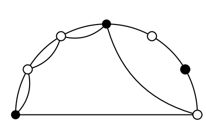


Corresponding sum in the coproduct:

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

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

ii) Diagrams with the first $\bullet$ marked:

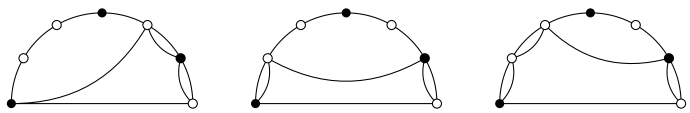


Corresponding sum in the coproduct:

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

The associated part of the Fourier expansion of $\mathbb{G}_{3,2}$ *is* $\mathbb{G}_{3,2}^{UR}(\tau) = \widehat{\mathrm{g}}(3) \cdot \zeta(2)$.

iii) Diagrams with the second • marked:



Corresponding sum in the coproduct:

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

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*

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

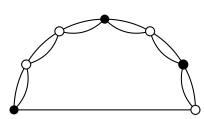
Also the associated part of the Fourier expansion is the most complicated one. We have

$$\mathbb{G}_{3,2}^{RU}(\tau) = \sum_{m>0} \Psi_{3,2}(m\tau)$$

and with (5.7) *we derived* $\Psi_{3,2}(x) = 3\Psi_2(x) \cdot \zeta(3) + \Psi_3(x) \cdot \zeta(2)$, *i.e.*

$$\mathbb{G}_{3,2}^{RU}(\tau) = 3\widehat{\mathrm{g}}(2) \cdot \zeta(3) + \widehat{\mathrm{g}}(3) \cdot \zeta(2)\,.$$

iv) Diagrams with both • marked:



Corresponding sum in the coproduct: $I(3,2) \otimes 1$. *The associated part of the Fourier expansion of* $\mathbb{G}_{3,2}$ *is* $\mathbb{G}_{3,2}^{UU}(\tau) = \widehat{\mathrm{g}}(3,2)$.

Summing all 4 *parts together we obtain for the coproduct*

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

and for the Fourier expansion of $\mathbb{G}_{2,3}(\tau)$*:*

$$\mathbb{G}_{3,2}(\tau) = \zeta(3,2) + 3\widehat{\mathrm{g}}(2)\zeta(3) + 2\widehat{\mathrm{g}}(3)\zeta(2) + \widehat{\mathrm{g}}(3,2)\,.$$

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

5.2.2 The q-series $\mathrm{g}^{\sqcup\!\sqcup}$

In this section we want to construct for $k_1,\dots,k_r \geq 1$ q-series $\mathrm{g}^{\sqcup\!\sqcup}(k_1,\dots,k_r)$ which satisfy the shuffle product formula. By this we mean that the following map is an $\mathbb{Q}$-algebra homomorphism

$$\begin{aligned}\mathrm{g}^{\sqcup\!\sqcup} : \mathfrak{H}^1_{\sqcup\!\sqcup} &\longrightarrow \mathbb{Q}[[q]]\\ z_{k_1}\dots z_{k_r} &\longmapsto \mathrm{g}^{\sqcup\!\sqcup}(k_1,\dots,k_r)\,.\end{aligned}$$

In smallest depths this means that we have for $k_1,k_2 \geq 1$ and $k = k_1+k_2$

$$\mathrm{g}^{\sqcup\!\sqcup}(k_1)\,\mathrm{g}^{\sqcup\!\sqcup}(k_2) = \sum_{j=1}^{k-1}\left(\binom{j-1}{k_1-1}+\binom{j-1}{k_2-1}\right)\mathrm{g}^{\sqcup\!\sqcup}(j,k-j)\,. \tag{5.10}$$

In Section 1.4 we saw in Proposition 1.30 that the q-series g satisfy a similar formula

$$\begin{aligned}\mathrm{g}(k_1)\,\mathrm{g}(k_2) = &\sum_{j=1}^{k-1}\left(\binom{j-1}{k_1-1}+\binom{j-1}{k_2-1}\right)\mathrm{g}(j,k-j)\\ &+\binom{k-2}{k_1-1}\left(q\frac{d}{dq}\frac{\mathrm{g}(k-2)}{k-2}-\mathrm{g}(k-1)\right)+\delta_{k_1,1}\delta_{k_2,1}\,\mathrm{g}(2)\,.\end{aligned} \tag{5.11}$$

Indeed we will see that the $\mathrm{g}^{\sqcup\!\sqcup}$ are given by the g if all indices are greater than 1. Comparing (5.10) and (5.11) we see that we could define the $g^{\sqcup\!\sqcup}$ for $k,k_1,k_2 \geq 1$ by

$$\begin{aligned}\mathrm{g}^{\sqcup\!\sqcup}(k) &= \mathrm{g}(k)\,,\\ \mathrm{g}^{\sqcup\!\sqcup}(k_1,k_2) &= \mathrm{g}(k_1,k_2)+\delta_{k_2,1}\cdot\frac{1}{2}\left(q\frac{d}{dq}\frac{\mathrm{g}(k_1-1)}{k_1-1}-\mathrm{g}(k_1)\right)\,.\end{aligned}$$

These series then satisfy the equation (5.10). For higher depths the derivatives $q\frac{d}{dq}$ will not be sufficient to correct the q-series g in order to get $\mathrm{g}^{\sqcup\!\sqcup}$. We will need to introduce the following double indexed version of g, on which we will focus in more detail in Section 5.3.

Definition 5.16. *For $k_1,\dots,k_r \geq 1$, $d_1,\dots,d_r \geq 0$ we define the q-series*

$$\begin{aligned}\mathrm{g}\binom{k_1,\dots,k_r}{d_1,\dots,d_r} &:= \sum_{m_1>\dots>m_r>0}\frac{m_1^{d_1}}{d_1!}\frac{P_{k_1}(q^{m_1})}{(1-q^{m_1})^{k_1}}\cdots\frac{m_r^{d_r}}{d_r!}\frac{P_{k_r}(q^{m_r})}{(1-q^{m_r})^{k_r}}\\ &= \sum_{\substack{m_1>\dots>m_r>0\\ n_1,\dots,n_r>0}}\frac{m_1^{d_1}}{d_1!}\frac{n_1^{k_1-1}}{(k_1-1)!}\cdots\frac{m_r^{d_r}}{d_r!}\frac{n_r^{k_r-1}}{(k_r-1)!}q^{m_1n_1+\dots+m_rn_r}\,.\end{aligned}$$

These generalize the q-series g, since by definition we have

$$\mathrm{g}\binom{k_1,\dots,k_r}{0,\dots,0} = \mathrm{g}(k_1,\dots,k_r)\,.$$

In depth one we can also see that these give the derivatives with respect to $q\frac{d}{dq}$, since

$$q\frac{d}{dq}\,\mathrm{g}(k) = q\frac{d}{dq}\sum_{\substack{m>0\\ n>0}}\frac{n^{k-1}}{(k-1)!}q^{mn} = \sum_{\substack{m>0\\ n>0}}\frac{mn^k}{(k-1)!}q^{mn} = k\sum_{\substack{m>0\\ n>0}}\frac{mn^k}{k!}q^{mn} = k\,\mathrm{g}\binom{k+1}{1}\,.$$

We will deal with the operator $q\frac{d}{dq}$ in more generality in Section 5.3. There we will also study the algebraic structure of these double indexed g and prove that they span the space of modified q-analogues, i.e. the space $\mathcal{Z}_q$ of modifed q-analogues (Eq. (1.31)) is spanned by the q-series $\mathrm{g}\binom{k_1,\dots,k_r}{d_1,\dots,d_r}$ (see Theorem 5.33).
We now want to construct the $\mathrm{g}^{\sqcup\!\sqcup}$ in general as elements in $\mathcal{Z}_q$ by defining them in terms of the double-indexed g. This will be done by using their generating series

$$\mathfrak{g}\binom{X_1,\dots,X_r}{Y_1,\dots,Y_r} := \sum_{\substack{k_1,\dots,k_r\geq 1\\ d_1,\dots,d_r\geq 0}} \mathrm{g}\binom{k_1,\dots,k_r}{d_1,\dots,d_r} X_1^{k_1-1}Y_1^{d_1}\cdots X_r^{k_r-1}Y_r^{d_r}\,.$$

Similar to Lemma 1.32 we obtain the following explicit expression.

Lemma 5.17. *We have*

$$\mathfrak{g}\binom{X_1,\dots,X_r}{Y_1,\dots,Y_r} = \sum_{m_1>\dots>m_r>0} e^{Y_1 m_1}\frac{e^{X_1}q^{m_1}}{1-e^{X_1}q^{m_1}}\cdots e^{Y_r m_r}\frac{e^{X_r}q^{m_r}}{1-e^{X_r}q^{m_r}}\,. \tag{5.12}$$

For $e_1,\dots,e_r \geq 1$ we generalize these generating series to the following

$$\mathcal{T}\begin{pmatrix} X_1, & \dots & ,X_r\\ Y_1, & \dots & ,Y_r\\ e_1, & \dots & ,e_r\end{pmatrix} = \sum_{m_1>\dots>m_r>0}\prod_{j=1}^{l} e^{m_jY_j}\left(\frac{e^{X_j}q^{m_j}}{1-e^{X_j}q^{m_j}}\right)^{e_j}\,. \tag{5.13}$$

In particular for $e_1=\dots=e_r=1$ these are the generating series of the g in (5.12). To show that the coefficients of these series are in $\mathcal{Z}_q$ for arbitrary e_j we need to define the differential operator $\mathcal{D}^Y_{e_1,\dots,e_r} := D_{Y_1,e_1}D_{Y_2,e_2}\dots D_{Y_r,e_r}$ 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 5.18. *The coefficients of* (5.13) *are in* $\mathcal{Z}_q$ *and we have*

$$\mathcal{D}^Y_{e_1,\dots,e_r}\mathfrak{g}\binom{X_1,\dots,X_r}{Y_1,\dots,Y_r} = \mathcal{T}\begin{pmatrix} Y_1+\dots+Y_r, & \dots & ,Y_1\\ X_r, X_{l-1}-X_r, & \dots & ,X_1-X_2\\ e_1, & \dots & ,e_r\end{pmatrix}.$$

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. □

Lemma 5.19. *Let A be an algebra spanned by elements $a_{k_1,\dots,k_r}$ with $k_1,\dots,k_r \in\geq 1$, let $H(X_1,\dots,X_r) = \sum_{k_j} a_{k_1,\dots,k_r}X_1^{k_1-1}\dots X_1^{k_r-1}$ be the generating functions of these elements and define for $f\in\mathbb{Q}[[X_1,\dots,X_r]]$*

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

Then the following two statements are equivalent.

i) The map $\mathfrak{H}^1_{ш} \to A$ *given by* $z_{k_1} \dots z_{k_j} \mapsto a_{k_1,\dots,k_r}$ *is an algebra homomorphism.*

ii) For all $r, s \geq 1$ *we have*

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

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* $(f\big|\sigma)(X_1, \dots, X_r) = f(X_{\sigma^{-1}(1)}, \dots, X_{\sigma^{-1}(r)})\,.$

Proof. This can be proven by induction over r together with Proposition 8 in [I]. □

Definition 5.20. *For* $k_1, \dots, k_r \geq 1$ *define* $\mathrm{g}^{ш}(k_1, \dots, k_r) \in \mathcal{Z}_q$ *as the coefficients of the following generating function*

$$\begin{aligned} H_{ш}(X_1, \dots, X_r) &= \sum_{k_1,\dots,k_r \geq 1} \mathrm{g}^{ш}(k_1, \dots, k_r) X_1^{k_1-1} \dots X_r^{k_r-1} \\ := \sum_{\substack{1 \leq m \leq r \\ i_1+\dots+i_m=r}} &\frac{1}{i_1! \dots i_m!} \mathcal{D}^Y_{i_1,\dots,i_m} \mathfrak{g}\begin{pmatrix} X_1, X_{i_m+1}, X_{i_{m-1}+i_m+1}, \dots, X_{i_2+\dots+i_m+1} \\ Y_1, \dots, Y_r \end{pmatrix}_{\Big|Y=0}. \end{aligned}$$

Theorem 5.21. *([B4, Thm. 5.7]) We have*

i) The $\mathrm{g}^{ш}(k_1, \dots, k_r)$ *satisfy the shuffle product formula, i.e.*

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

ii) For $k_1 \geq 1$, $k_2, \dots, k_r \geq 2$ *we have* $\mathrm{g}^{ш}(k_1, \dots, k_r) = \mathrm{g}(k_1, \dots, k_r)$.

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 $A = \left\{ \binom{y}{n} \mid n \geq 1\,, y \in Y_{\mathbb{Z}} \right\}$, 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 $\binom{y_1,\dots,y_r}{n_1,\dots,n_r}$. 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 $*_\diamond$ (see Section 2.3) and therefore obtain a quasi-shuffle algebra $(\mathbb{Q}\langle A \rangle, *_\diamond)$. It is easy to see that the map $(\mathbb{Q}\langle A \rangle, *_\diamond) \to \varinjlim_j \mathbb{Q}[[q]][[X_1, \dots, X_j, Y_1, \dots, Y_j]]$ given by

$$\begin{pmatrix} y_1, \dots, y_r \\ n_1, \dots, n_r \end{pmatrix} \longmapsto \mathcal{T}\begin{pmatrix} 0,\dots,0 \\ y_1,\dots,y_r \\ n_1,\dots,n_r \end{pmatrix}$$

is an algebra homomorphism. Using now Theorem 2.28 the series h defined by the exponential map

$$h(X_1, \dots, X_r) = \sum_{\substack{1 \leq m \leq n \\ i_1+\dots+i_m=n}} \frac{1}{i_1! \dots i_m!} \mathcal{T}\begin{pmatrix} 0, & \dots & ,0 \\ Y_1, & \dots & ,Y_m \\ i_1, & \dots & ,i_m \end{pmatrix},$$

where $Y_j = X_{i_1+\dots+i_{j-1}} + \dots + X_{i_1+\dots+i_j}$ with $X_0 := 0$, satisfies 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 $H_{ш}(X_1, \dots, X_r) := h(X_r, X_{l-1} - X_r, \dots, X_1 - X_2)$ and by the same argument as in Theorem 4.3 in [BT] it is

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

Combining the definition of h and $H_{\sqcup\!\sqcup}$ we observe that $H_{\sqcup\!\sqcup}(X_1, \dots, X_r)$ equals

$$\sum_{\substack{1\leq m\leq n\\ i_1+\dots+i_m=n}} \frac{1}{i_1!\dots i_m!}\mathcal{T}\begin{pmatrix} 0, & \dots & ,0 \\ X_{r-i_1+1}, X_{r-i_1-i_2+1}-X_{r-i_1+1}, & \dots & ,X_1-X_{r-i_1-\dots-i_{m-1}+1} \\ i_1, & \dots & ,i_m \end{pmatrix}.$$

We now apply Proposition 5.18 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 $X_2, \dots, X_r$ appear, is the one with $i_1 = \dots = i_m = 1$ which is exactly $\mathrm{g}(k_1, \dots, k_r)X^{k_1-1} \dots X_r^{k_r-1}$. Therefore the q-series $\mathrm{g}^{\sqcup\!\sqcup}(k_1, \dots, k_r)$ where $k_2, \dots, k_r \geq 2$ are given by $\mathrm{g}(k_1, \dots, k_r)$. □

For small depths we obtain the following explicit expressions for $\mathrm{g}^{\sqcup\!\sqcup}$.

Corollary 5.22. *We have* $\mathrm{g}(k_1)^{\sqcup\!\sqcup} = \mathrm{g}(k_1)$ *and for* $r = 2, 3, 4$ *the* $\mathrm{g}^{\sqcup\!\sqcup}(k_1, \dots, k_r)$ *are given by*[11]

i) $$\mathrm{g}^{\sqcup\!\sqcup}(k_1,k_2) = \mathrm{g}(k_1,k_2) + \delta_{k_2,1}\cdot\frac{1}{2}\left(\mathrm{g}\binom{k_1}{1} - \mathrm{g}(k_1)\right),$$

ii) $$\begin{aligned}\mathrm{g}^{\sqcup\!\sqcup}(k_1,k_2,k_3) = \mathrm{g}(k_1,k_2,k_3) &+ \delta_{k_3,1}\cdot\frac{1}{2}\left(\mathrm{g}\binom{k_1,k_2}{0,1} - \mathrm{g}(k_1,k_2)\right)\\ &+ \delta_{k_2,1}\cdot\frac{1}{2}\left(\mathrm{g}\binom{k_1,k_3}{1,0} - \mathrm{g}\binom{k_1,k_3}{0,1} - \mathrm{g}(k_1,k_3)\right)\\ &+ \delta_{k_2\cdot k_3,1}\cdot\frac{1}{6}\left(\mathrm{g}\binom{k_1}{2} - \frac{3}{2}\mathrm{g}\binom{k_1}{1} + \mathrm{g}(k_1)\right),\end{aligned}$$

iii) $$\begin{aligned}\mathrm{g}^{\sqcup\!\sqcup}(k_1,k_2,k_3,k_4) &= \mathrm{g}(k_1,k_2,k_3,k_4) + \delta_{k_4,1}\cdot\frac{1}{2}\left(\mathrm{g}\binom{k_1,k_2,k_3}{0,0,1} - \mathrm{g}(k_1,k_2,k_3)\right)\\ &+\delta_{k_3,1}\cdot\frac{1}{2}\left(\mathrm{g}\binom{k_1,k_2,k_4}{0,1,0} - \mathrm{g}\binom{k_1,k_2,k_4}{0,0,1} + \mathrm{g}(k_1,k_2,k_4)\right)\\ &+\delta_{k_2,1}\cdot\frac{1}{2}\left(\mathrm{g}\binom{k_1,k_3,k_4}{1,0,0} - \mathrm{g}\binom{k_1,k_3,k_4}{0,1,0} + \mathrm{g}(k_1,k_3,k_4)\right)\\ &+\delta_{k_2\cdot k_4,1}\cdot\frac{1}{4}\left(\mathrm{g}\binom{k_1,k_3}{1,1} - 2\,\mathrm{g}\binom{k_1,k_3}{0,2} - \mathrm{g}\binom{k_1,k_3}{1,0} + \mathrm{g}(k_1,k_3)\right)\\ &+\delta_{k_3\cdot k_4,1}\cdot\frac{1}{6}\left(\mathrm{g}\binom{k_1,k_2}{0,2} - \frac{3}{2}\mathrm{g}\binom{k_1,k_2}{0,1} + \mathrm{g}(k_1,k_2)\right)\\ &+\delta_{k_2\cdot k_3,1}\cdot\frac{1}{6}\left(\mathrm{g}\binom{k_1,k_4}{0,2} - \mathrm{g}\binom{k_1,k_4}{1,1} + \frac{3}{2}\mathrm{g}\binom{k_1,k_4}{0,1} + \mathrm{g}\binom{k_1,k_4}{2,0} - \frac{3}{2}\mathrm{g}\binom{k_1,k_4}{1,0} + \mathrm{g}(k_1,k_4)\right)\\ &+\delta_{k_2\cdot k_3\cdot k_4,1}\cdot\frac{1}{24}\left(\mathrm{g}\binom{k_1}{3} - 2\,\mathrm{g}\binom{k_1}{2} + \frac{11}{6}\mathrm{g}\binom{k_1}{1} - \mathrm{g}(k_1)\right).\end{aligned}$$

Proof. This follows by calculating the coefficients of the series $H_{\sqcup\!\sqcup}$. □

5.2.3 Shuffle regularized multiple Eisenstein series

In this section, we present the definition of shuffle regularized multiple Eisenstein series as it was done in [BT]. We use the observation of the previous section and use the coproduct Δ_G of formal iterated integrals to define these series. As mentioned in Remark 5.14 we can equip the space $\mathfrak{H}^1$ with the

[11] Here $\delta_{a,b}$ again denotes the Kronecker delta, i.e $\delta_{a,b}$ is 1 for $a = b$ and 0 otherwise.

coproduct Δ_G instead of working with the space $\mathcal{I}^1$. In analogy to the map $\zeta^{\shuffle} : \mathfrak{H}^1_{\shuffle} \to \mathcal{Z}$ of shuffle regularized multiple zeta values, the map

$$\widehat{\mathrm{g}}^{\shuffle} : \mathfrak{H}^1_{\shuffle} \to \mathbb{Q}[2\pi i][\![q]\!]$$

defined on the generators $z_{k_1} \dots z_{k_r}$ by

$$\widehat{\mathrm{g}}^{\shuffle}(z_{k_1} \dots z_{k_r}) := (-2\pi i)^{k_1+\dots+k_r}\, \mathrm{g}^{\shuffle}(k_1, \dots, k_r)\,,$$

is also an algebra homomorphism by Theorem 5.21. With this we can give the definition of $\mathbb{G}^{\shuffle}$ ([BT]).

Definition 5.23. *For $k_1, \dots, k_r \geq 1$ define the* **shuffle regularized multiple Eisenstein series** *by*

$$\mathbb{G}^{\shuffle}_{k_1,\dots,k_r}(\tau) := m\left((\widehat{\mathrm{g}}^{\shuffle} \otimes \zeta^{\shuffle}) \circ \Delta_G\big(z_{k_1} \dots z_{k_r}\big)\right)\,,$$

where m denotes the multiplication given by $m : a \otimes b \mapsto a \cdot b$ and $\zeta^{\shuffle}$ denotes shuffle regularized multiple zeta values (Definition 2.34 with $T = 0$).

We can view $\mathbb{G}^{\shuffle}$ as an algebra homomorphism $\mathbb{G}^{\shuffle} : \mathfrak{H}^1_{\shuffle} \to \mathcal{Z}[\pi \mathrm{i}][\![\mathrm{q}]\!]$ such that the following diagram commutes

$$\begin{tikzcd}
\mathfrak{H}^1_{\shuffle} \arrow[r, "\Delta_G"] \arrow[d, "\mathbb{G}^{\shuffle}"'] & \mathfrak{H}^1_{\shuffle} \otimes \mathfrak{H}^1_{\shuffle} \arrow[d, "\widehat{\mathrm{g}}^{\shuffle} \otimes \zeta^{\shuffle}"] \\
\mathcal{Z}[\pi \mathrm{i}][\![\mathrm{q}]\!] & \mathbb{Q}[2\pi i][\![q]\!] \otimes \mathcal{Z} \arrow[l, "m"]
\end{tikzcd}$$

Theorem 5.24. *([BT, Thm. 1.1, 1.2]) For all $k_1, \dots, k_r \geq 1$ the shuffle regularized multiple Eisenstein series $\mathbb{G}^{\shuffle}_{k_1,\dots,k_r}$ 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, i.e. they can be written as

$$\mathbb{G}^{\shuffle}_{k_1,\dots,k_r}(\tau) = \zeta^{\shuffle}(k_1, \dots, k_r) + \sum_{n=1}^{\infty} a_n q^n\,. \qquad (a_n \in \mathcal{Z}[\pi i] = \mathcal{Z} + \pi i \mathcal{Z}) \tag{5.14}$$

ii) They satisfy the shuffle product formula.

iii) For integers $k_1, \dots, k_r \geq 2$ they equal the multiple Eisenstein series

$$\mathbb{G}^{\shuffle}_{k_1,\dots,k_r}(\tau) = \mathbb{G}_{k_1,\dots,k_r}(\tau)$$

and therefore satisfy the stuffle product formula 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 5.15, holds in general. It also shows that the shuffle regularized multiple Eisenstein series satisfy the stuffle product formula in many cases. Though the exact failure of the stuffle product of these series is unknown so far.

5.2.4 Stuffle regularized multiple Eisenstein series

Now we want to construct the stuffle regularized multiple Eisenstein series. Motivated by the calculation of the Fourier expansion of multiple Eisenstein series, we consider the following construction.

Construction 5.25. Given a $\mathbb{Q}$-algebra $(A,\cdot)$ and a family of homomorphism

$$\{w \mapsto f_w(m)\}_{m\geq 1}$$

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

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

where $\ell(w)$ 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 5.26. *([B4, Prop. 6.8]) For all $M\geq 1$ the assignment $w\mapsto F_w(M)$, described above, determines an algebra homomorphism from $\mathfrak{H}^1_*$ to $(A,\cdot)$. In particular $\{w\mapsto F_w(m)\}_{m\geq 1}$ is again a family of homomorphism as used in Construction 5.25.*

For a word $w = z_{k_1}\dots z_{k_r}\in\mathfrak{H}^1$ we also write in the following $f_{k_1,\dots,k_r}(m) := f_w(m)$ and similarly $F_{k_1,\dots,k_r}(M) := F_w(M)$.

Example 5.27. *Let $f_w(m)$ be as in Construction 5.25. In small depths the F_w are given by*

$$F_{k_1}(M) = \sum_{M>m_1>0} f_{k_1}(m_1)\,,\quad F_{k_1,k_2}(M) = \sum_{M>m_1>0} f_{k_1,k_2}(m_1) + \sum_{M>m_1>m_2>0} f_{k_1}(m_1)f_{k_2}(m_2)$$

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

$$\begin{aligned}
&F_{k_1}(M)\cdot F_{k_2}(M) = \sum_{M>m_1>0} f_{k_1}(m_1)\cdot \sum_{M>m_2>0} f_{k_2}(m_2)\\
&= \sum_{M>m_1>m_2>0} f_{k_1}(m_1)f_{k_2}(m_2) + \sum_{M>m_2>m_1>0} f_{k_2}(m_2)f_{k_1}(m_1) + \sum_{M>m_1>0} f_{k_1}(m_1)f_{k_2}(m_1)\\
&= \sum_{M>m_1>m_2>0} f_{k_1}(m_1)f_{k_2}(m_2) + \sum_{M>m_2>m_1>0} f_{k_2}(m_2)f_{k_1}(m_1)\\
&+ \sum_{M>m_1>0} \left(f_{k_1,k_2}(m_1) + f_{k_2,k_1}(m_1) + f_{k_1+k_2}(m_1)\right)\\
&= F_{k_1,k_2}(M) + F_{k_2,k_1}(M) + F_{k_1+k_2}(M)\,.
\end{aligned}$$

Let us now give an explicit example for maps f_w in which we are interested. Recall (Definition 5.5) that for integers $k_1,\dots,k_r\geq 2$ we defined the multitangent function by

$$\Psi_{k_1,\dots,k_r}(x) = \sum_{\substack{n_1>\dots>n_r\\ n_j\in\mathbb{Z}}} \frac{1}{(x+n_1)^{k_1}\cdots(x+n_r)^{k_r}}.$$

In [Bo], where these functions were introduced, the author uses the notation $\mathcal{T}e^{k_1,\dots,k_r}(x)$ which corresponds to our notation $\Psi_{k_1,\dots,k_r}(x)$. It was shown there that the series $\Psi_{k_1,\dots,k_r}(x)$ converges absolutely when $k_1, \dots, k_r \geq 2$. These functions fulfill (for the cases they are defined) the stuffle product. As explained in Section 5 the multitangent functions appear in the calculation of the Fourier expansion of the multiple Eisenstein series $\mathbb{G}_{k_1,\dots,k_r}$, for example in depth two we have

$$\begin{aligned}\mathbb{G}_{k_1,k_2}(\tau) =& \zeta(k_1,k_2) + \zeta(k_1) \sum_{m_1>0} \Psi_{k_2}(m_1\tau) + \sum_{m_1>0} \Psi_{k_1,k_2}(m_1\tau) \\ &+ \sum_{m_1>m_2>0} \Psi_{k_1}(m_1\tau)\Psi_{k_2}(m_2\tau)\,.\end{aligned}$$

One nice result of [Bo] is a regularization of the multitangent function to get a definition of $\Psi_{k_1,\dots,k_r}(x)$ for all $k_1, \dots, k_r \geq 1$. We will use this result together with the above construction to recover the Fourier expansion of the multiple Eisenstein series.

Theorem 5.28. *([Bo]) For all $k_1, \dots, k_r \geq 1$ there exist holomorphic functions $\Psi_{k_1,\dots,k_r}$ 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 $k_1, \dots, k_r \geq 2$ the $\Psi_{k_1,\dots,k_r}$ are given by the multitangent functions in Definition 5.5.

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

$$\Psi_1(\tau) = \frac{\pi}{\tan(\pi\tau)} = (-2\pi i)\left(\frac{1}{2} + \sum_{n>0} q^n\right)$$

and for $k \geq 2$ by

$$\Psi_k(\tau) = \frac{(-2\pi i)^k}{(k-1)!} \sum_{n>0} n^{k-1} q^n\,.$$

iv) (Reduction into monotangent function) Every $\Psi_{k_1,\dots,k_r}(\tau)$ can be written as a $\mathcal{Z}$-linear combination of monotangent functions. There are explicit $\epsilon_{i,k}^{k_1,\dots,k_r} \in \mathcal{Z}$ s.th.

$$\Psi_{k_1,\dots,k_r}(\tau) = \delta^{k_1,\dots,k_r} + \sum_{i=1}^{l} \sum_{k=1}^{k_i} \epsilon_{i,k}^{k_1,\dots,k_r} \Psi_k(\tau)\,,$$

where $\delta^{k_1,\dots,k_r} = \frac{(\pi i)^r}{r!}$ if $k_1 = \cdots = k_r = 1$ and r even and $\delta^{k_1,\dots,k_r} = 0$ otherwise. For $k_1 > 1$ and $k_r > 1$ 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]. □

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. We have seen in Proposition 5.7 that for $k_1, \dots, k_r \geq 2$ we have

$$\widehat{\mathrm{g}}(k_1, \dots, k_r) = \sum_{m_1>\cdots>m_r>0} \Psi_{k_1}(m_1\tau) \dots \Psi_{k_r}(m_r\tau)\,.$$

For $w \in \mathfrak{H}^1$ we now use the Construction 5.25 with $A = \mathbb{C}[\![q]\!]$ and the family of homomorphism $\{w \mapsto \Psi_w(n\tau)\}_{n\geq 1}$ (See Theorem 5.28 i)) to define

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

From Proposition 5.26 it follows that for all $M \geq 1$ 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 (See [HI]) that the space $(\mathbb{Q}\langle A\rangle, *_\diamond, \Delta_H)$ has the structure of a Hopf algebra. With this, we try to mimic the definition of the $\mathbb{G}^{ш}$ and use the coproduct structure on the space $(\mathfrak{H}^1, *, \Delta_H)$ to define for $M \geq 0$ the function $\mathbb{G}^{*,M}$ and then take the limit $M \to \infty$ to obtain the stuffle regularized multiple Eisenstein series. For this, we consider the following diagram

$$\begin{tikzcd}
(\mathfrak{H}^1, *) \arrow[r, "\Delta_H"] \arrow[d, "\mathbb{G}^{*,M}"'] & (\mathfrak{H}^1, *) \otimes (\mathfrak{H}^1, *) \arrow[d, "\mathrm{g}^{*,M} \otimes \zeta^*"] \\
\mathbb{C}[\![q]\!] & \mathbb{C}[\![q]\!] \otimes \mathcal{Z} \arrow[l, "m"]
\end{tikzcd}$$

with the above algebra homomorphism $\mathrm{g}^{*,M} : (\mathfrak{H}^1, *) \to \mathbb{C}[\![q]\!]$ and the map ζ^* for stuffle regularized multiple zeta values given in Definition 2.34 (with $T = 0$).

Definition 5.29. *For integers $k_1, \dots, k_r \geq 1$ and $M \geq 1$, we define the q-series $\mathbb{G}^{*,M}_{k_1,\dots,k_r} \in \mathbb{C}[\![q]\!]$ as the image of the word $w = z_{k_1}\dots z_{k_r} \in \mathfrak{H}^1$ under the algebra homomorphism $(\mathrm{g}^{*,M} \otimes \zeta^*) \circ \Delta_H$:*

$$\mathbb{G}^{*,M}_{k_1,\dots,k_r}(\tau) := m\left((\mathrm{g}^{*,M} \otimes \zeta^*) \circ \Delta_H(w)\right) \in \mathbb{C}[\![q]\!]\,.$$

For $k_1, \dots, k_r \geq 2$ the limit

$$\mathbb{G}^{*}_{k_1,\dots,k_r}(\tau) := \lim_{M\to\infty} \mathbb{G}^{*,M}_{k_1,\dots,k_r}(\tau) \tag{5.15}$$

exists and we have $\mathbb{G}_{k_1,\dots,k_r} = \mathbb{G}^{*}_{k_1,\dots,k_r} = \mathbb{G}^{ш}_{k_1,\dots,k_r}$ ([B4, Prop. 6.13]).

Remark 5.30. The limit in (5.15) exists in the cases $k_1 \geq 2$ and $k_2, \dots, k_r \geq 1$ as explained in Remark 6.14 in [B4]. For $k_1 = 1$ this limit does not exist, since the monotangent function Ψ_1 has a constant term in its Fourier expansion. It is an open problem to give a definition of $\mathbb{G}^*$ for all indices.

Theorem 5.31. *([B4]) For all $k_1, \dots, k_r \geq 1$ and $M \geq 1$ the $\mathbb{G}^{*,M}_{k_1,\dots,k_r} \in \mathbb{C}[\![q]\!]$ have the following properties:*

i) Their product can be expressed in terms of the stuffle product.

ii) In the case where the limit $\mathbb{G}^{*}_{k_1,\dots,k_r} := \lim_{M\to\infty} \mathbb{G}^{*,M}_{k_1,\dots,k_r}$ exists, the functions $\mathbb{G}^{*}_{k_1,\dots,k_r}$ are elements in $\mathcal{Z}[\pi \mathrm{i}][\![\mathrm{q}]\!]$.

iii) For $k_1, \dots, k_r \geq 2$ the $\mathbb{G}^{*}_{k_1,\dots,k_r}$ exist and equal the classical multiple Eisenstein series

$$\mathbb{G}_{k_1,\dots,k_r}(\tau) = \mathbb{G}^{*}_{k_1,\dots,k_r}(\tau)\,.$$

5.2.5 Double shuffle relations for regularized multiple Eisenstein series

By Theorem 5.24 we know that the product of two shuffle regularized multiple Eisenstein series $\mathbb{G}^{ш}_{k_1,\dots,k_r}$ with $k_1,\dots,k_r \geq 1$ can be expressed by using the shuffle product formula. This means we can for example replace every ζ by $\mathbb{G}^{ш}$ in the shuffle product (Example1.10) of multiple zeta values and obtain

$$\mathbb{G}^{ш}_2 \cdot \mathbb{G}^{ш}_3 = \mathbb{G}^{ш}_{2,3} + 3\mathbb{G}^{ш}_{3,2} + 6\mathbb{G}^{ш}_{4,1} \,. \tag{5.16}$$

Due to Theorem 5.24 iii) we know that $\mathbb{G}^{ш}_{k_1,\dots,k_r} = \mathbb{G}_{k_1,\dots,k_r}$ whenever $k_1,\dots,k_r \geq 2$. Since the product of two multiple Eisenstein series $\mathbb{G}_{k_1,\dots,k_r}$ can be expressed using the stuffle product formula we also have

$$\begin{aligned} \mathbb{G}^{ш}_2 \cdot \mathbb{G}^{ш}_3 &= \mathbb{G}_2 \cdot \mathbb{G}_3 = \mathbb{G}_{2,3} + \mathbb{G}_{3,2} + \mathbb{G}_5 \\ &= \mathbb{G}^{ш}_{2,3} + \mathbb{G}^{ш}_{3,2} + \mathbb{G}^{ш}_5 \,. \end{aligned} \tag{5.17}$$

Combining (5.16) and (5.17) we obtain the relation $\mathbb{G}^{ш}_5 = 2\mathbb{G}^{ш}_{3,2} + 6\mathbb{G}^{ш}_{4,1}$. In the following we will call these relations, i.e. the relations obtained by writing the product of two $\mathbb{G}^{ш}_{k_1,\dots,k_r}$ with $k_1,\dots,k_r \geq 2$ 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 $\zeta(k_1,\dots,k_r)$ in two different ways whenever $k_1 \geq 2$ and $k_2,\dots,k_r \geq 1$. A natural question therefore is, in which cases the $\mathbb{G}^{ш}$ 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 [B4, Example 6.15] it is shown that $\mathbb{G}^{ш}_{2,1,2} = \mathbb{G}^{*}_{2,1,2}$, $\mathbb{G}^{ш}_{2,1} = \mathbb{G}^{*}_{2,1}$, $\mathbb{G}^{ш}_{2,2,1} = \mathbb{G}^{*}_{2,2,1}$ and $\mathbb{G}^{ш}_{4,1} = \mathbb{G}^{*}_{4,1}$. Since the product of two $\mathbb{G}^*$ can be expressed using the stuffle product we obtain

$$\begin{aligned} \mathbb{G}^{ш}_2 \cdot \mathbb{G}^{ш}_{2,1} &= \mathbb{G}^{*}_2 \cdot \mathbb{G}^{*}_{2,1} \\ &= \mathbb{G}^{*}_{2,1,2} + 2\mathbb{G}^{*}_{2,2,1} + \mathbb{G}^{*}_{4,1} + \mathbb{G}^{*}_{2,3} \\ &= \mathbb{G}^{ш}_{2,1,2} + 2\mathbb{G}^{ш}_{2,2,1} + \mathbb{G}^{ш}_{4,1} + \mathbb{G}^{ш}_{2,3} \,. \end{aligned} \tag{5.18}$$

Using also the shuffle product to express $\mathbb{G}^{ш}_2 \cdot \mathbb{G}^{ш}_{2,1}$ 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 $\mathbb{G}^{ш}$ can be written in terms of stuffle products.

5.3 Double indexed q-analogues of MZV

In this Section, we want to study the double indexed version of g, which we defined in Definition 5.16 for $k_1, \dots, k_r \geq 1$, $d_1, \dots, d_r \geq 0$ by

$$\mathrm{g}\binom{k_1, \dots, k_r}{d_1, \dots, d_r} := \sum_{m_1 > \dots > m_r > 0} \frac{m_1^{d_1}}{d_1!} \frac{P_{k_1}(q^{m_1})}{(1-q^{m_1})^{k_1}} \cdots \frac{m_r^{d_r}}{d_r!} \frac{P_{k_r}(q^{m_r})}{(1-q^{m_r})^{k_r}}$$
$$= \sum_{\substack{m_1 > \dots > m_r > 0 \\ n_1, \dots, n_r > 0}} \frac{m_1^{d_1}}{d_1!} \frac{n_1^{k_1-1}}{(k_1-1)!} \cdots \frac{m_r^{d_r}}{d_r!} \frac{n_r^{k_r-1}}{(k_r-1)!} q^{m_1 n_1 + \dots + m_r n_r} .$$

By $k_1 + \dots + k_r + d_1 + \dots + d_r$ we denote its weight and by r its depth. These q-series are also modified q-analogues of multiple zeta values.

Proposition 5.32. *For $k_1 \geq d_1 + 2$ and $k_j \geq d_j + 1$ for $j = 2, \dots, r$ we have*

$$\lim_{q \to 1} (1-q)^{k_1 + \dots + k_r} \, \mathrm{g}\binom{k_1, \dots, k_r}{d_1, \dots, d_r} = \frac{1}{d_1! \cdots d_r!} \zeta(k_1 - d_1, k_2 - d_2, \dots, k_r - d_r) .$$

Proof. This proof is similar to the proof of Proposition 1.26, since we have

$$\lim_{q \to 1} (1-q)^k \frac{m^d P_k(q^m)}{(1-q^m)^k} = \lim_{q \to 1} \frac{m^d P_k(q^m)}{[m]_q^k} = \frac{m^d P_k(1)}{m^k} = \frac{1}{m^{k-d}} .$$

□

In fact these q-series span the space of all modified q-analogues, which we defined in Section 1.4 by

$$\mathcal{Z}_q := \mathbb{Q} + \left\langle \zeta_q(k_1, \dots, k_r; Q_1, \dots, Q_r) \;\middle|\; r \geq 1,\, k_1, \dots, k_r \geq 1,\, \deg(Q_j) \leq k_j \right\rangle_{\mathbb{Q}} .$$

Here we defined the $\zeta_q(k_1, \dots, k_r; Q_1, \dots, Q_r)$ for $k_1, \dots, k_r \geq 1$ and polynomials $Q_1(X) \in X\mathbb{Q}[X]$ and $Q_2(X) \dots, Q_r(X) \in \mathbb{Q}[X]$ by

$$\zeta_q(k_1, \dots, k_r; Q_1, \dots, Q_r) = \sum_{m_1 > \dots > m_r > 0} \frac{Q_1(q^{m_1}) \dots Q_r(q^{m_r})}{(1-q^{m_1})^{k_1} \cdots (1-q^{m_r})^{k_r}} .$$

These series are modified q-analogues of $\zeta(k_1, \dots, k_r)$, since we have for $k_1 \geq 2$

$$\lim_{q \to 1} (1-q)^{k_1 + \dots + k_r} \zeta_q(k_1, \dots, k_r; Q_1, \dots, Q_r) = Q_1(1) \dots Q_r(1) \cdot \zeta(k_1, \dots, k_r) .$$

Theorem 5.33. *The space $\mathcal{Z}_q$ of modifed q-analogues is spanned by the q-series $\mathrm{g}\binom{k_1, \dots, k_r}{d_1, \dots, d_r}$, i.e.*

$$\mathcal{Z}_q = \mathbb{Q} + \left\langle \mathrm{g}\binom{k_1, \dots, k_r}{d_1, \dots, d_r} \;\middle|\; k_1, \dots, k_r \geq 1, d_1, \dots, d_r \geq 0 \right\rangle_{\mathbb{Q}} .$$

Proof. We give a variation of the proof as given in [BK2]. First we show the inclusion '$\subseteq$' , i.e. that every $\zeta_q(k_1, \dots, k_r; Q_1, \dots, Q_r)$ can be written in terms of g. For all $k \geq 1$ we have $P_{k-1}(1) = 1$ and $P_{k-1}(0) = 0$ and therefore the polynomials $P_{j-1}(X)(1-X)^{k-j}$ with $j = 1, \dots, k$ form a basis of the space $\{Q \in X\mathbb{Q}[X] \mid \deg Q \leq k\}$. In particular for every polynomial Q in this space there exist coefficients $\alpha_j \in \mathbb{Q}$ with

$$\frac{Q(X)}{(1-X)^k} = \sum_{j=1}^{k} \alpha_j \frac{P_{j-1}(X)}{(1-X)^j} . \tag{5.19}$$

Therefore we just need to see what happens if one of the $Q_2, \dots, Q_r$ has a constant term. Without loss of generality we can focus on the cases $Q_i(X) = 1$ for a $2 \leq i \leq r$. Since for all $k \geq 1$ we have

$$\frac{1}{(1-X)^k} = 1 + \sum_{m=1}^{k} \frac{X}{(1-X)^m} ,$$

we can write

$$\sum_{n_1 > \dots > n_r > 0} \prod_{j=1}^{r} \frac{Q_j(q^{n_j})}{(1-q^{n_j})^{s_j}} = \sum_{n_1 > \dots > n_r > 0} \prod_{\substack{j=1\\ j\neq i}}^{r} \frac{Q_j(q^{n_j})}{(1-q^{n_j})^{s_j}} + \sum_{\substack{n_1 > \dots > n_r > 0\\ 1 \leq m \leq s_i}} \frac{q^{n_i}}{(1-q^{n_i})^m} \prod_{\substack{j=1\\ j\neq i}}^{r} \frac{Q_j(q^{n_j})}{(1-q^{n_j})^{s_j}} .$$

For the the second sum on the right-hand side we can again use (5.19). For the first sum we obtain (by setting $n_{l+1} = 0$)

$$\sum_{n_1 > \dots > n_r > 0} \prod_{\substack{j=1\\ j\neq i}}^{r} \frac{Q_j(q^{n_j})}{(1-q^{n_j})^{s_j}} = \sum_{n_1 > \dots > n_{i-1} > n_{i+1} > \dots > n_r > 0} (n_{i-1} - n_{i+1} - 1) \prod_{\substack{j=1\\ j\neq i}}^{r} \frac{Q_j(q^{n_j})}{(1-q^{n_j})^{s_j}} .$$

Repeating this for all $2 \leq i \leq r$ with $Q_i(X) = 1$ we obtain linear combinations of g, from which we deduce '$\subseteq$'. To prove '$\supseteq$' we first define for $m \geq 0$ the polynomials $p_m(n)$ by $p_0(n) = 1$ and

$$p_m(n) = \sum_{n > N_1 > \dots > N_m > 0} 1 = \binom{n-1}{m} . \tag{5.20}$$

The $p_m(n)$ is a polynomial in n of degree m and therefore we can always find $c_m(r) \in \mathbb{Q}$ with $n^r = \sum_{m=0}^{r} c_m(r)\, p_m(n)$. The idea is now to replace $n_j^{r_j}$ in the definition of g by $\sum_{m_j=0}^{r_j} c_{m_j}(r_j)\, p_{m_j}(n_j)$ and then use (5.20) to get sums which can be written in terms of the ζ_q. We illustrate this in the depth two case from which the general case becomes clear. We have with $\kappa = (k_1-1)!(k_2-1)!d_1!d_2!$

$$\begin{aligned}
\kappa \cdot \mathrm{g}\binom{k_1, k_2}{d_1, d_2} &= \sum_{n_1 > n_2 > 0} \frac{n_1^{d_1} P_{k_1-1}(q^{n_1})}{(1-q^{n_1})^{k_1}} \frac{n_2^{d_2} P_{k_2-1}(q^{n_2})}{(1-q^{n_2})^{k_2}} \\
&= \sum_{0 \leq m_2 \leq d_2} c_{m_2}(d_2) \sum_{n_1 > n_2 > N_1 > \dots > N_{m_2} > 0} \frac{n_1^{d_1} P_{k_1-1}(q^{n_1})}{(1-q^{n_1})^{k_1}} \frac{P_{k_2-1}(q^{n_2})}{(1-q^{n_2})^{k_2}} \\
&= \sum_{\substack{0 \leq m_1 \leq d_1\\ 0 \leq m_2 \leq d_2}} c_{m_1}(d_1) c_{m_2}(d_2) \sum_{\substack{n_1 > n_2 > N_1 > \dots > N_{m_2} > 0\\ n_1 > N_1' > \dots > N_{m_1}' > 0}} \frac{P_{k_1-1}(q^{n_1})}{(1-q^{n_1})^{k_1}} \frac{P_{k_2-1}(q^{n_2})}{(1-q^{n_2})^{k_2}} .
\end{aligned}$$

Now considering all the possible shuffles, and possible equalities of the N and the N' it is clear that this sum can be written as a linear combination of ζ_q by interpreting appearing 1 as $(1-q^N)(1-q^N)^{-1}$. For general depth r the idea is the same and therefore we obtain '$\supseteq$'. □

Since the double indexed g generalize the single indexed g we clearly have $\mathcal{G} \subset \mathcal{Z}_q$. In Proposition 2.20 we saw that the following spaces

$$\mathcal{G}^{\geq 2} = \Big\langle \, \mathrm{g}(k_1, \dots, k_r) \;\big|\; r \geq 0,\, k_1, \dots, k_r \geq 2 \Big\rangle_{\mathbb{Q}} ,$$
$$\mathcal{G}^{\mathrm{ev}} = \Big\langle \, \mathrm{g}(k_1, \dots, k_r) \;\big|\; r \geq 0,\, k_1, \dots, k_r \geq 2 \text{ even} \Big\rangle_{\mathbb{Q}} ,$$

are also subalgebras of $\mathcal{G}$. Further we saw in Proposition 2.25 that the algebra of quasi-modular forms (with rational coefficients) $\widetilde{\mathcal{M}}^{\mathbb{Q}} = \mathbb{Q}[\mathrm{g}(2), \mathrm{g}(4), \mathrm{g}(6)]$ is a subalgebra of $\mathcal{G}^{\mathrm{ev}}$. Combining all this we obtain the following inclusions of $\mathbb{Q}$-algebras

$$\mathcal{M}^{\mathbb{Q}} \subset \widetilde{\mathcal{M}}^{\mathbb{Q}} \subset \mathcal{G}^{\mathrm{ev}} \subset \mathcal{G}^{\geq 2} \subset \mathcal{G} \subset \mathcal{Z}_q \,. \tag{5.21}$$

We will see that g form a nice generating set of modified q-analogues since they behave well under the operator $q\frac{d}{dq}$, and they satisfy the partition relations, which we can use to describe an analogue of double shuffle relations for them. Conjecturally these relations give all relations among elements in $\mathcal{Z}_q$ and by (5.21) they are sufficient to prove any relation among (quasi-)modular forms.

5.3.1 The operator $q\frac{d}{dq}$

In this section we will study the operator $q\frac{d}{dq}$. We saw already that the space of quasi modular forms $\widetilde{\mathcal{M}}^{\mathbb{Q}}$ is closed under this operator. In this section we will see that this also the case for $\mathcal{Z}_q$ and $\mathcal{G}$. First notice that this operator on a q-series is given as follows

$$q\frac{d}{dq} \sum_{n=1}^{\infty} a_n q^n = \sum_{n=1}^{\infty} n\, a_n q^n \,.$$

Applying this to g therefore gives

$$\begin{aligned} q\frac{d}{dq}\, \mathrm{g}\binom{k_1, \dots, k_r}{d_1, \dots, d_r} &= \sum_{\substack{m_1 > \dots > m_r > 0 \\ n_1, \dots, n_r > 0}} \frac{m_1^{d_1}}{d_1!} \frac{n_1^{k_1-1}}{(k_1-1)!} \cdots \frac{m_r^{d_r}}{d_r!} \frac{n_r^{k_r-1}}{(k_r-1)!} (m_1 n_1 + \dots + m_r n_r) q^{m_1 n_1 + \dots + m_r n_r} \,. \\ &= \sum_{j=1}^{r} (d_j + 1) k_j \, \mathrm{g}\binom{k_1, \dots, k_j + 1, \dots, k_r}{d_1, \dots, d_j + 1, \dots, d_r} . \end{aligned} \tag{5.22}$$

In particular we obtain the following:

Proposition 5.34. *The space $\mathcal{Z}_q$ is closed under $q\frac{d}{dq}$.*

Proof. This follows by Theorem 5.33 together with (5.22). □

In [BK1] it was shown that also the subspace $\mathcal{G}$ generated by $\mathrm{g}(k_1, \dots, k_r)$ is closed under $q\frac{d}{dq}$. This is not obvious, since by (5.22) we have

$$q\frac{d}{dq}\, \mathrm{g}(k_1, \dots, k_r) = \sum_{j=1}^{r} k_j \, \mathrm{g}\binom{k_1, \dots, k_j + 1, \dots, k_r}{0, \dots, 1, \dots, 0} .$$

A priori it is not clear why the right-hand side can also be written in terms of single indexed g. In the following we will give a proof of this fact by using generating series. For this we consider the following series (which is a special case of the $\mathcal{T}\binom{\vdots}{\vdots}$ in (5.13))

$$H\binom{n_1,\dots,n_r}{X_1,\dots,X_r} = \sum_{m_1>\dots>m_r>0} e^{m_1 X_1}\left(\frac{q^{m_1}}{1-q^{m_1}}\right)^{n_1} \cdots e^{m_r X_r}\left(\frac{q^{m_r}}{1-q^{m_r}}\right)^{n_r}.$$

By Lemma 1.32 we have the following relationship between H and the generating series of $\mathrm{g}(k_1,\dots,k_r)$

$$H\binom{1,\dots,1}{X_1,\dots,X_r} = \mathfrak{g}(X_1+\dots+X_r, X_1+\dots+X_{r-1},\dots,X_1)\,.$$

Also notice that the H satisfy the stuffle product formula, e.g.

$$H\binom{n_1}{X_1}H\binom{n_1}{X_1} = H\binom{n_1,n_2}{X_1,X_2} + H\binom{n_2,n_1}{X_2,X_1} + H\binom{n_1+n_2}{X_1+X_2}.$$

Therefore we get

$$\begin{aligned}\mathfrak{g}(X_1)\mathfrak{g}(X_2) = H\binom{1}{X_1}H\binom{1}{X_2} &= H\binom{1,1}{X_1,X_2} + H\binom{1,1}{X_2,X_1} + H\binom{2}{X_1+X_2} \\ &= \mathfrak{g}(X_1+X_2,X_1) + \mathfrak{g}(X_1+X_2,X_2) + H\binom{2}{X_1+X_2}.\end{aligned} \tag{5.23}$$

Now we use $q\frac{d}{dq}\frac{q^m}{1-q^m} = m\left(\frac{q^m}{1-q^m}\right)^2 + m\frac{q^m}{1-q^m}$ to obtain

$$\begin{aligned}q\frac{d}{dq}\mathfrak{g}(X) = q\frac{d}{dq}H\binom{1}{X} = q\frac{d}{dq}\sum_{m>0} e^{mX}\frac{q^m}{1-q^m} &= \sum_{m>0} me^{mX}\left(\frac{q^m}{1-q^m}\right)^2 + \sum_{m>0} me^{mX}\frac{q^m}{1-q^m} \\ = \frac{d}{dY}\left(H\binom{2}{X+Y} + H\binom{1}{X+Y}\right)_{Y=0}.\end{aligned} \tag{5.24}$$

Combining (5.23) and (5.24) we obtain

$$q\frac{d}{dq}\mathfrak{g}(X) = \frac{d}{dY}\big(\mathfrak{g}(X)\mathfrak{g}(Y) - \mathfrak{g}(X+Y,X) - \mathfrak{g}(X+Y,Y) + \mathfrak{g}(X+Y)\big)_{Y=0}.$$

Since $\frac{d}{dY}\mathfrak{g}(Y)_{Y=0} = \mathrm{g}(2)$ the above formula somehow states that $q\frac{d}{dq}\,\mathrm{g}(k)$ measures, up to lower weight terms, the failure of the shuffle product formula for $\mathrm{g}(k)\,\mathrm{g}(2)$. Also notice that this is just a special case of the shuffle product formula

$$\begin{aligned}\mathrm{g}(k_1)\,\mathrm{g}(k_2) = &\sum_{j=1}^{k-1}\left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1}\right)\mathrm{g}(j,k-j) \\ &+ \binom{k-2}{k_1-1}\left(q\frac{d}{dq}\frac{\mathrm{g}(k-2)}{k-2} - \mathrm{g}(k-1)\right) + \delta_{k_1,1}\delta_{k_2,1}\,\mathrm{g}(2)\,.\end{aligned}$$

The same strategy works in arbitrary depths, and we obtain the following.

Theorem 5.35. *The space $\mathcal{G}$ is closed under $q\frac{d}{dq}$.*

Proof. With the same idea as above we obtain

$$\begin{aligned} q\frac{d}{dq}\mathfrak{g}(X_1,\dots,X_r) &= \mathfrak{g}(X_1,\dots,X_r)\,\mathrm{g}(2) \\ &\quad - \frac{d}{dY}\left(\sum_{j=0}^{r-1}\mathfrak{g}(X_1+Y,\dots,X_{j+1}+Y,X_{j+1},\dots,X_r)+\mathfrak{g}(X_1+Y,\dots,X_r+Y,Y)\right)\Bigg|_{Y=0} \\ &\quad + \frac{d}{dY}\left(\sum_{j=1}^{r}\mathfrak{g}(X_1+Y,\dots,X_{r-j+1}+Y,X_{r-j+2},\dots,X_r)\right)\Bigg|_{Y=0} \end{aligned}$$

from which we obtain the statement. □

By Lemma 5.19 we can also interpret the right-hand side here as the measure of the failure of the shuffle product formula for $\mathrm{g}(k_1,\dots,k_r)\,\mathrm{g}(2)$ (up to lower weight terms coming from the last sum).

Conjecture 5.36. *The space $\mathcal{G}^{\geq 2}$ is closed under $q\frac{d}{dq}$.*

For this conjecture, not much is known so far. Just the depth one case and some special cases are proven so far.

Proposition 5.37. *For $k \geq 1$ we have*

$$\begin{aligned} \frac{d}{dq}\,\mathrm{g}(k) =& (2k-1)\,\mathrm{g}(k+2) - \sum_{j=2}^{k}(k+j-1)\,\mathrm{g}(k+2-j,j) - \mathrm{g}(2,k) \\ &+ \sum_{j=2}^{k}\frac{B_{k+2-j}}{(k+2-j)!}(3k-j+1)\,\mathrm{g}(j) + (-1)^k\frac{B_k}{k!}\,\mathrm{g}(2)\,. \end{aligned}$$

In particular $\frac{d}{dq}\,\mathrm{g}(k) \in \mathcal{G}^{\geq 2}$ for $k \geq 2$.

Proof. This follows from Proposition 1.30 and can also be found in [B5]. □

One motivation for Conjecture 5.36 is the connection to multiple Eisenstein series. In Theorem 5.4 we saw that the multiple Eisenstein series $\mathbb{G}_{k_1,\dots,k_r}$ can be written as a $\mathbb{C}$-linear combination of g. In particular we have the following

$$\mathbb{C} + \langle \mathbb{G}(k_1,\dots,k_r) \mid r \geq 1, k_1,\dots,k_r \geq 2\rangle_{\mathbb{C}} = \mathbb{C}\otimes\mathcal{G}^{\geq 2}\,.$$

In particular Conjecture 5.36 would imply that also the space of multiple Eisenstein series is closed under $q\frac{d}{dq} = \frac{1}{2\pi i}\frac{d}{d\tau}$. Again this fact can be shown in depth one as a consequence of Proposition 5.37.

Theorem 5.38. *For $k \geq 2$ we have*

$$(2\pi i)\frac{d}{d\tau}\mathbb{G}_k(\tau) = (2k-1)\mathbb{G}_{k+2}(\tau) - \sum_{j=2}^{k}(k+j-1)\mathbb{G}_{k+2-j,j}(\tau) - \mathbb{G}_{2,k}(\tau)\,.$$

Proof. This is a consequence of Proposition 5.37 together with the formula for the Fourier expansion of the double Eisenstein series given in Proposition 5.10. □

One does not expect that the space $\mathcal{G}^{\mathrm{ev}}$ is closed under $q\frac{d}{dq}$, since it seems already be the case that $q\frac{d}{dq}\,\mathrm{g}(4,2) \notin \mathcal{G}^{\mathrm{ev}}$. Summarizing everything we get the following overview.

$$
\begin{tikzcd}
\mathcal{M}^{\mathbb{Q}} \arrow[r, hook] \arrow[r, bend right, "q\frac{d}{dq}"'] & \widetilde{\mathcal{M}}^{\mathbb{Q}} \arrow[r, hook] \arrow[loop above, "q\frac{d}{dq}"] & \mathcal{G}^{\mathrm{ev}} \arrow[r, hook] \arrow[r, bend right, dashed, "q\frac{d}{dq}?"'] & \mathcal{G}^{\geq 2} \arrow[r] \arrow[loop above, dashed, "q\frac{d}{dq}?"] & \mathcal{G} \arrow[r, hook] \arrow[loop above, "q\frac{d}{dq}"] & \mathcal{Z}_q \arrow[loop above, "q\frac{d}{dq}"]
\end{tikzcd}
$$

Figure 5: Overview of the (conjectured) behavior of the operator $q\frac{d}{dq}$.

5.3.2 Partition relation

In this section we will introduce a family of linear relations among the g, which follows immediately when viewing the coefficient of q^N as a sum over all partitions of N. By a partition of a natural number N with r parts we denote a representation of N as a sum of r 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 $(m,n) \in \mathbb{N}^r \times \mathbb{N}^r$ where the m_j's are the r distinct numbers in the partition and the n_j's count their appearance in the sum. The above partition of 15 is therefore given by the tuple $(m,n) = ((4,3,2,1),(2,1,1,2))$. By $P_r(N)$ we denote all **partitions of N with r parts** and write

$$P_r(N) := \{(m,n) \in \mathbb{N}^r \times \mathbb{N}^r \mid N = m_1 n_1 + \cdots + m_r n_r \text{ and } m_1 > \cdots > m_r > 0\}$$

On the set $P_r(N)$ we have an involution given by the conjugation ρ of partitions which can be obtained by reflecting the corresponding Young diagram across the main diagonal.

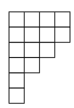
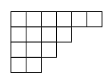
$((4,3,2,1),(2,1,1,2)) =$  $\xrightarrow{\rho}$  $= ((6,4,3,2),(1,1,1,1))$

Figure 6: 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.

On the set $P_r(N)$ the conjugation ρ is explicitly given by $\rho((m,n)) = (m',n')$ where $m'_j = n_1 + \cdots + n_{r-j+1}$ and $n'_j = m_{r-j+1} - m_{r-j+2}$ with $m_{r+1} := 0$, i.e.

$$\rho : \begin{pmatrix} m_1, \ldots, m_r \\ n_1, \ldots, n_r \end{pmatrix} \longmapsto \begin{pmatrix} n_1 + \cdots + n_r, \ldots, n_1 + n_2, n_1 \\ m_r, m_{r-1} - m_r, \ldots, m_1 - m_2 \end{pmatrix}. \tag{5.25}$$

We can interpret the coefficient of q^N in g as a sum over all partitions of N, since we have

$$\begin{aligned}
\mathrm{g}\begin{pmatrix} k_1, \ldots, k_r \\ d_1, \ldots, d_r \end{pmatrix} &= \sum_{\substack{m_1 > \cdots > m_r > 0 \\ n_1, \ldots, n_r > 0}} \frac{m_1^{d_1}}{d_1!} \frac{n_1^{k_1 - 1}}{(k_1-1)!} \cdots \frac{m_r^{d_r}}{d_r!} \frac{n_r^{k_r-1}}{(k_r-1)!} q^{m_1 n_1 + \cdots + m_r n_r} \\
&= \sum_{N>0} \left(\sum_{(m,n) \in P_r(N)} \frac{m_1^{d_1}}{d_1!} \frac{n_1^{k_1-1}}{(k_1-1)!} \cdots \frac{m_r^{d_r}}{d_r!} \frac{n_r^{k_r-1}}{(k_r-1)!} \right) q^N
\end{aligned}$$

The coefficients are given by a sum over all elements in $P_r(N)$ and therefore it is invariant under the action of ρ, which implies relations among g. These relations can be written down nicely in terms of generating series. Recall that we denote these by

$$\mathfrak{g}\binom{X_1,\dots,X_r}{Y_1,\dots,Y_r} := \sum_{\substack{k_1,\dots,k_r\geq 1\\ d_1,\dots,d_r\geq 0}} \mathrm{g}\binom{k_1,\dots,k_r}{d_1,\dots,d_r} X_1^{k_1-1}Y_1^{d_1}\cdots X_r^{k_r-1}Y_r^{d_r}\,.$$

Lemma 5.39. *For $m \geq 1$ set*

$$E_m(X) := e^{mX} \qquad \text{and} \qquad L_m(X) := \frac{e^X q^m}{1-e^X q^m} \in \mathbb{Q}[[q,X]]\,.$$

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

$$\begin{aligned}\mathfrak{g}\binom{X_1,\dots,X_r}{Y_1,\dots,Y_r} &= \sum_{m_1>\dots>m_r>0}\prod_{j=1}^{r} E_{m_j}(Y_j)L_{m_j}(X_j)\\ &= \sum_{m_1>\dots>m_r>0}\prod_{j=1}^{r} E_{m_j}(X_{r+1-j}-X_{r+2-j})L_{m_j}(Y_1+\dots+Y_{r-j+1})\end{aligned}$$

(with $X_{r+1} := 0$).

Proof. This follows by a similar change of variables as it was done in Lemma 1.32 which are exactly given by (5.25). ☐

As a direct consequence of Lemma 5.39 we obtain the following.

Theorem 5.40. *(Partition relation) We have*[12]

$$\mathfrak{g}\binom{X_1,\dots,X_r}{Y_1,\dots,Y_r} = \mathfrak{g}\binom{Y_1+\dots+Y_r,\dots,Y_1+Y_2,Y_1}{X_r,X_{r-1}-X_r,\dots,X_1-X_2}\,. \tag{5.26}$$

Comparing the coefficients of both sides yields linear relations among g, which are exactly those coming from the above interpretation as a sum over all partitions of N for the coefficient of q^N.

Corollary 5.41. *(Partition relation in depth one and two) For $k,k_1,k_2 \geq 2$ and $d,d_1,d_2 \geq 0$ we have the following relations in length one and two*

$$\begin{aligned}\mathrm{g}\binom{k}{d} &= \mathrm{g}\binom{d+1}{k-1}\,,\\ \mathrm{g}\binom{k_1,k_2}{d_1,d_2} &= \sum_{\substack{0\leq j\leq d_1\\ 0\leq i\leq k_2-1}} (-1)^i \binom{k_1-1+i}{i}\binom{d_2+j}{j}\mathrm{g}\binom{d_2+1+j\,,d_1+1-j}{k_2-1-i\,,k_1-1+i}\,.\end{aligned}$$

5.3.3 Double shuffle relations for g

In the following we will describe the algebraic structure of the g. For this we will again use the notion of quasi-shuffle algebras. Recall that we introduced the Quasi-shuffle algebra $(\mathbb{Q}\langle A_z\rangle, \hat{*})$, where the product $\hat{*}$ is the quasi-shuffle product induced by the following product on $\mathbb{Q}A_z$

$$z_{k_1}\hat{\diamond} z_{k_2} = z_{k_1+k_2} + \sum_{j=1}^{k_1+k_2-1}\left(\lambda^j_{k_1,k_2}+\lambda^j_{k_2,k_1}\right)z_j\,, \tag{5.27}$$

[12]The generating series are an examples of a **bimould**. In the language of moulds the partition relation (5.26) states that the bimould of the generating series $\mathfrak{g}$ is swap invariant.

where the rational numbers $\lambda^j_{k_1,k_2}$ are given by

$$\lambda^j_{k_1,k_2} = (-1)^{k_2-1}\binom{k_1+k_2-1-j}{k_1-j}\frac{B_{k_1+k_2-j}}{(k_1+k_2-j)!}\,.$$

We then viewed g as an algebra homomorphism from $(\mathbb{Q}\langle A_z\rangle, \hat{*})$ to $\mathcal{G}$, by sending $z_{k_1}\cdots z_{k_r}$ to $\mathrm{g}(k_1,\dots,k_r)$. This setup can be generalized in an obvious way for the double indexed version of g. For this we first define the double indexed version of $A_z = \{z_1, z_2, \dots\}$ by

$$A_z^{\mathrm{bi}} := \left\{ \begin{bmatrix} k \\ d \end{bmatrix} \mid k \geq 1, d \geq 0 \right\}.$$

We can view A_z as a subset of A_z^{bi} by identifying z_k with $\left[\begin{smallmatrix} k \\ 0 \end{smallmatrix}\right]$. On $\mathbb{Q}A_z^{\mathrm{bi}}$ we define the following product

$$\begin{bmatrix} k_1 \\ d_1 \end{bmatrix} \hat{\diamond} \begin{bmatrix} k_2 \\ d_2 \end{bmatrix} := \binom{d_1+d_2}{d_1}\begin{bmatrix} k_1+k_2 \\ d_1+d_2 \end{bmatrix} + \binom{d_1+d_2}{d_1}\sum_{j=1}^{k_1+k_2-1}\left(\lambda^j_{k_1,k_2}+\lambda^j_{k_2,k_1}\right)\begin{bmatrix} j \\ d_1+d_2 \end{bmatrix}. \tag{5.28}$$

Clearly (5.28) reduces to (5.27) in the case $d_1 = d_2 = 0$. One can check that this is again a commutative and associative product and we therefore obtain a quasi-shuffle algebra $(\mathbb{Q}\langle A_z^{\mathrm{bi}}\rangle, \hat{*})$ (Theorem 2.17). For convenience we write for a word in the alphabet A_z^{bi}

$$\begin{bmatrix} k_1,\dots,k_r \\ d_1,\dots,d_r \end{bmatrix} := \begin{bmatrix} k_1 \\ d_1 \end{bmatrix}\cdots\begin{bmatrix} k_r \\ d_r \end{bmatrix}.$$

Again we can view g as a $\mathbb{Q}$-linear map defined as follows

$$\begin{aligned} \mathrm{g} : \mathbb{Q}\langle A_z^{\mathrm{bi}}\rangle &\longrightarrow \mathcal{Z}_q \\ \begin{bmatrix} k_1,\dots,k_r \\ d_1,\dots,d_r \end{bmatrix} &\longmapsto \mathrm{g}\begin{pmatrix} k_1,\dots,k_r \\ d_1,\dots,d_r \end{pmatrix}. \end{aligned}$$

Proposition 5.42. *The map* g *is an algebra homomorphism from* $(\mathbb{Q}\langle A_z^{bi}\rangle, \hat{*})$ *to* $\mathcal{Z}_q$.

Proof. This is a direct consequence of Lemma 2.18 and

$$\begin{aligned} \frac{m^{d_1}}{d_1!}\frac{P_{k_1}(X)}{(1-X)^{k_1}}\cdot\frac{m^{d_2}}{d_2!}\frac{P_{k_2}(X)}{(1-X)^{k_2}} =& \binom{d_1+d_2}{d_1}\frac{m^{d_1+d_2}}{(d_1+d_2)!}\frac{P_{k_1+k_2}(X)}{(1-X)^{k_1+k_2}} \\ &+ \binom{d_1+d_2}{d_1}\sum_{j=1}^{k_1+k_2-1}\left(\lambda^j_{k_1,k_2}+\lambda^j_{k_2,k_1}\right)\frac{m^{d_1+d_2}}{(d_1+d_2)!}\frac{P_j(X)}{(1-X)^j}, \end{aligned}$$

which follows from Lemma 1.28. □

The product $\hat{*}$ on $\mathbb{Q}\langle A_z^{\mathrm{bi}}\rangle$ can be viewed as the analogue for the stuffle product. In the following we want to describe a product $\hat{ш}$, which gives an analogue of the shuffle product. To define this product we will use the partition relations described in the previous subsection. Consider the following genering series of words in A_z^{bi}

$$\mathfrak{w}\begin{pmatrix} X_1,\dots,X_r \\ Y_1,\dots,Y_r \end{pmatrix} := \sum_{\substack{k_1,\dots,k_r\geq 1 \\ d_1,\dots,d_r\geq 0}} \begin{bmatrix} k_1,\dots,k_r \\ d_1,\dots,d_r \end{bmatrix} X_1^{k_1-1}Y_1^{d_1}\cdots X_r^{k_r-1}Y_r^{d_r} \in \mathbb{Q}\langle A_z^{\mathrm{bi}}\rangle[[X_1,Y_1,\dots,X_r,Y_r]]\,.$$

Definition 5.43. *We define the $\mathbb{Q}$-linear map $P : \mathbb{Q}\langle A_z^{bi}\rangle \to \mathbb{Q}\langle A_z^{bi}\rangle$ on the generators by*

$$\sum_{\substack{k_1,\dots,k_r\geq 1\\ d_1,\dots,d_r\geq 0}} P\left(\begin{bmatrix} k_1,\dots,k_r \\ d_1,\dots,d_r\end{bmatrix}\right) X_1^{k_1-1}Y_1^{d_1}\cdots X_r^{k_r-1}Y_r^{d_r} := \mathfrak{w}\binom{Y_1+\dots+Y_r,\dots,Y_1+Y_2,Y_1}{X_r, X_{r-1}-X_r,\dots,X_1-X_2}.$$

Notice that P is an involution and that it corresponds exactly to the partition relation, i.e. we have for example $P\left(\left[\begin{smallmatrix}k\\d\end{smallmatrix}\right]\right) = \left[\begin{smallmatrix}d+1\\k+1\end{smallmatrix}\right]$. In particular we get the following.

Proposition 5.44. *The map* g *is P-invariant, i.e. we have $\mathrm{g}(P(w)) = \mathrm{g}(w)$ for all $w \in \mathbb{Q}\langle A_z^{bi}\rangle$.*

Using the map P we can define a new product on the space $\mathbb{Q}\langle A_z^{\mathrm{bi}}\rangle$ as follows.

Definition 5.45. *We define the product $\hat{⧢}$ for $w, v \in \mathbb{Q}\langle A_z^{bi}\rangle$ by*

$$w \,\hat{⧢}\, v := P\left(P(w) \,\hat{*}\, P(v)\right).$$

Proposition 5.46. *Equipped with the product $\hat{⧢}$ the space $\mathbb{Q}\langle A_z^{bi}\rangle$ becomes a commutative $\mathbb{Q}$-algebra and* g *gives a $\mathbb{Q}$-algebra homomorphism $\mathrm{g} : (\mathbb{Q}\langle A_z^{bi}\rangle, \hat{⧢}) \to \mathcal{Z}_q$.*

Proof. The first statement follows direclty from the commutativity and associativity of $\hat{*}$. The second statement follows from the P-invariance of g. ☐

Theorem 5.47. *(Double shuffle relations for* g*). For all $w, v \in \mathbb{Q}\langle A_z^{bi}\rangle$ we have*

$$\mathrm{g}(w \,\hat{⧢}\, v - w \,\hat{*}\, v) = 0\,.$$

Proof. This is a consequence of Proposition 5.42 and 5.46. ☐

We will now give an example, which indicated why $\hat{⧢}$ could be seen as an analogue of the shuffle product.

Example 5.48. *First we give the following example for the map P (Using Corollary 5.41)*

$$P\left(\begin{bmatrix}1,1\\1,2\end{bmatrix}\right) = \begin{bmatrix}3,2\\0,0\end{bmatrix} + 3\begin{bmatrix}4,1\\0,0\end{bmatrix},$$
$$P\left(\begin{bmatrix}1,1\\2,1\end{bmatrix}\right) = \begin{bmatrix}2,3\\0,0\end{bmatrix} + 2\begin{bmatrix}3,2\\0,0\end{bmatrix} + 3\begin{bmatrix}4,1\\0,0\end{bmatrix}.$$

Using this we obtain

$$\begin{aligned}\begin{bmatrix}2\\0\end{bmatrix} \hat{⧢} \begin{bmatrix}3\\0\end{bmatrix} &= P\left(P\left(\begin{bmatrix}2\\0\end{bmatrix}\right) \hat{*}\, P\left(\begin{bmatrix}3\\0\end{bmatrix}\right)\right) = P\left(\begin{bmatrix}1\\1\end{bmatrix} \hat{*} \begin{bmatrix}1\\2\end{bmatrix}\right)\\ &= P\left(\begin{bmatrix}1,1\\1,2\end{bmatrix} + \begin{bmatrix}1,1\\2,1\end{bmatrix} + 3\begin{bmatrix}2\\3\end{bmatrix} - 3\begin{bmatrix}1\\3\end{bmatrix}\right)\\ &= \begin{bmatrix}2,3\\0,0\end{bmatrix} + 3\begin{bmatrix}3,2\\0,0\end{bmatrix} + 6\begin{bmatrix}4,1\\0,0\end{bmatrix} + 3\begin{bmatrix}4\\1\end{bmatrix} - 3\begin{bmatrix}4\\0\end{bmatrix}.\end{aligned}$$

Together with

$$\begin{bmatrix}2\\0\end{bmatrix} \hat{*} \begin{bmatrix}3\\0\end{bmatrix} = \begin{bmatrix}2,3\\0,0\end{bmatrix} + \begin{bmatrix}3,2\\0,0\end{bmatrix} + \begin{bmatrix}5\\0\end{bmatrix} - \frac{1}{12}\begin{bmatrix}3\\0\end{bmatrix}$$

this gives the following linear relation among the q-series g

$$\mathrm{g}\binom{5}{0} = 2\,\mathrm{g}\binom{3,2}{0,0} + 6\,\mathrm{g}\binom{4,1}{0,0} + \frac{1}{12}\,\mathrm{g}\binom{3}{0} - 3\,\mathrm{g}\binom{4}{0} + 3\,\mathrm{g}\binom{4}{1}. \tag{5.29}$$

Notice that this gives exactly the same formula as in Example 1.31, but the new setup also allows to consider these products in higher depths.

In general it was shown in [B2] and [Zu3] that the $\hat{\sqcup\!\sqcup}$ corresponds to the classical stuffle & shuffle product of multiple zeta values after considering the limit $q \to 1$.

In the case of multiple zeta values, we saw that conjecturally the extended double shuffle relations give all relations. A similar conjecture exists for the modified q-analogues g given as follows.

Conjecture 5.49. *All linear relations among* g *are a consequence of the double shuffle relations and the partition relation, i.e. we have*

$$\ker(\mathrm{g}) = \langle w \,\hat{\sqcup\!\sqcup}\, v - w \,\hat{*}\, v \mid w, v \in \mathbb{Q}\langle A_z^{bi}\rangle\rangle_{\mathbb{Q}} + \langle P(w) - w \mid w \in \mathbb{Q}\langle A_z^{bi}\rangle\rangle_{\mathbb{Q}}\,.$$

In (5.29), we see that the double indexed $\mathrm{g}\binom{4}{1}$ can be written in terms of single indexed g. As mentioned in the beginning, this seems to be the case in general, i.e., any double indexed g can be expressed in the original (single indexed) g and therefore $\mathcal{Z}_q = \mathcal{G}$.

Conjecture 5.50. *We have* $\mathcal{Z}_q = \mathcal{G}$*. More precisely any* $\mathrm{g}\binom{k_1,\dots,k_r}{d_1,\dots,d_r}$ *can be expressed as a linear combination of* $\mathrm{g}(s_1,\dots,s_l)$ *with* $1 \le l \le r + d_1 + \dots + d_r$ *and* $s_1 + \dots + s_l \le k_1 + \dots + k_r + d_1 + \dots + d_r$*.*

Not much is known so far for this conjecture. It has been checked up to weight 9 (using the double shuffle relations) and it is proven for all weights in depths one (as a consequence of Theorem 5.35). Besides this just a few special cases are known in depths two ([B4]).

Example 5.51. *Using the double shuffle relations for* g *one can show that*

$$\begin{aligned} \mathrm{g}\binom{3,2}{1,0} =& -\frac{1}{8}\,\mathrm{g}(6) - \mathrm{g}(5,1) + \frac{5}{2}\,\mathrm{g}(4,2) - \frac{3}{4}\,\mathrm{g}(4,1,1) - \frac{5}{4}\,\mathrm{g}(3,2,1) \\ & - \frac{1}{1440}\,\mathrm{g}(2) + \frac{7}{96}\,\mathrm{g}(3) - \frac{1}{3}\,\mathrm{g}(4) - \frac{7}{48}\,\mathrm{g}(3,1) + \frac{1}{2}\,\mathrm{g}(5) + \frac{3}{4}\,\mathrm{g}(4,1) + \frac{5}{8}\,\mathrm{g}(3,2)\,. \end{aligned} \tag{5.30}$$

We saw in Proposition 5.32, that $\mathrm{g}\binom{3,2}{1,0}$ can be viewed as an q-analogue of $\zeta(2,2)$, since

$$\lim_{q\to 1}(1-q)^5\,\mathrm{g}\binom{3,2}{1,0} = \zeta(2,2)\,.$$

But according to Conjecture 5.50 the q-series is actually something of weight 6 and not 5. But clearly $\lim_{q\to1}(1-q)^6\,\mathrm{g}\binom{3,2}{1,0} = 0$, and therefore (5.30) implies a relation among multiple zeta values given by

$$\zeta(6) = 20\zeta(4,2) - 8\zeta(5,1) - 6\zeta(4,1,1) - 10\zeta(3,2,1)\,.$$

In general almost all double indexed $\mathrm{g}\binom{k_1,\dots,k_r}{d_1,\dots,d_r}$ vanish when considering the limit $\lim_{q\to1}(1-q)^{k_1+\dots+k_r+d_1+\dots+d_r}$. Conjecture 5.50 therefore implies relations among multiple zeta values, which conjectureally give all relations among multiple zeta values.

Multiple zeta values and modular forms
Exercises

Topics in Mathematical Science III, Nagoya University (Spring 2020)

Deadline: Middle of August 2020.

Exercise 1.

i) Prove Proposition 1.9, i.e. show that for $k_1, k_2 \geq 2$ we have

$$\zeta(k_1)\zeta(k_2) = \sum_{j=2}^{k_1+k_2-1} \left(\binom{j-1}{k_1-1} + \binom{j-1}{k_2-1} \right) \zeta(j, k_1+k_2-j)\,.$$

For this you can use (without a proof) the partial fraction expansion ($a, b \geq 1$)

$$\frac{1}{x^a y^b} = \sum_{j=1}^{a+b-1} \left(\frac{\binom{j-1}{a-1}}{(x+y)^j y^{a+b-j}} + \frac{\binom{j-1}{b-1}}{(x+y)^j x^{a+b-j}} \right),$$

which can be proven by induction on a and b.

ii) Use i) together with $\zeta(k_1)\zeta(k_2) = \zeta(k_1,k_2) + \zeta(k_2,k_1) + \zeta(k_1+k_2)$ to prove the relation

$$\zeta(7) = 4\zeta(3,4) + 3\zeta(4,3) - 2\zeta(5,2)\,.$$

Exercise 2.

i) Show that Conjecture 1.12 together with Proposition 1.11 would imply that all multiple zeta values (except for $\zeta(\emptyset) = 1$) are transcendental.

ii) Show that Conjecture 1.16 (Hoffman) would imply Conjecture 1.13 (Zagier).

iii) Show that Conjecture 1.21 (Broadhurst-Kreimer) would imply Conjecture 1.13 (Zagier).

Exercise 3. We defined for $k \geq 1$ the Eulerian polynomials $P_k(X)$ and the power series $R_k(X)$ by

$$R_k(X) = \frac{P_k(X)}{(1-X)^k} = \sum_{d>0} \frac{d^{k-1}}{(k-1)!} X^d\,.$$

i) Prove Lemma 1.24, i.e. show that we have $P_k(0) = 0$ and $P_k(1) = 1$ for all $k \geq 1$.

ii) Prove Lemma 1.28, i.e. show that for all $k_1, k_2 \geq 1$

$$R_{k_1}(X) \cdot R_{k_2}(X) = R_{k_1+k_2}(X) + \sum_{j=1}^{k_1+k_2-1} \left(\lambda^j_{k_1,k_2} + \lambda^j_{k_2,k_1} \right) R_j(X)\,,$$

where the rational numbers $\lambda^j_{k_1,k_2}$ are given by

$$\lambda^j_{k_1,k_2} = (-1)^{k_2-1} \binom{k_1+k_2-1-j}{k_1-j} \frac{B_{k_1+k_2-j}}{(k_1+k_2-j)!}\,,$$

and where we use the convention $\binom{n}{k} = 0$ for $k < 0$.

Exercise 4. Define for even $k \geq 4$ the normalized Eisenstein series E_k by $E_k = \zeta(k)^{-1}\mathbb{G}_k \in \mathcal{M}_k$. Show that we have

$$E_k = 1 - \frac{2k!}{B_k}\,\mathrm{g}(k)$$

and **give two different proofs** of the identity

$$E_4^2 = E_8 \tag{5.31}$$

between the Eisenstein series

$$E_4 = 1 + 240\sum_{n=1}^{\infty}\sigma_3(n)q^n \quad \text{and} \quad E_8 = 1 + 480\sum_{n=1}^{\infty}\sigma_7(n)q^n\,.$$

i) Analytic proof of (5.31): Use the theory of modular forms, i.e. use Theorem 1.19 and 1.20.

ii) Combinatorial proof of (5.31): You are just allowed to use Proposition 1.29 and 1.30 .

Exercise 5.

i) Prove Lemma 1.32, i.e. show that

$$\mathfrak{g}(X_1,\dots,X_r) = \sum_{k_1,\dots,k_r\geq 1} g(k_1,\dots,k_r)X_1^{k_1-1}\cdots X_r^{k_r-1}$$

can be written in the following two ways

$$\begin{aligned}\mathfrak{g}(X_1,\dots,X_r) &= \sum_{m_1>\dots>m_r>0}\frac{e^{X_1}q^{m_1}}{1-e^{X_1}q^{m_1}}\cdots\frac{e^{X_r}q^{m_r}}{1-e^{X_r}q^{m_r}}\\ &= \sum_{m_1>\dots>m_r>0}\frac{e^{m_1X_r}q^{m_1}}{1-q^{m_1}}\frac{e^{m_2(X_{r-1}-X_r)}q^{m_2}}{1-q^{m_2}}\cdots\frac{e^{m_r(X_1-X_2)}q^{m_r}}{1-q^{m_r}}\,.\end{aligned}$$

ii) Show equation (1.29), i.e. show that we have

$$\sum_{m>0}e^{mX}\frac{q^m}{(1-q^m)^2} = \mathrm{g}(2) + q\frac{d}{dq}\sum_{k\geq 1}\mathrm{g}(k)\frac{X^k}{k}\,.$$

iii) Show that Propositions 1.29 and 1.30 are a consequence of Proposition 1.33.

Exercise 6.

i) Calculate (2.2) by hand, i.e. show

$$\zeta(2,3) = \int_0^1\frac{dt_1}{t_1}\int_0^{t_1}\frac{dt_2}{1-t_2}\int_0^{t_2}\frac{dt_3}{t_3}\int_0^{t_3}\frac{dt_4}{t_4}\int_0^{t_5}\frac{dt_5}{1-t_5}\,.$$

without using Corollary 2.4.

ii) Prove Proposition 2.12, i.e. show for that for any $w, u \in \mathfrak{H}^1$ and $M \geq 1$ we have

$$\zeta_M(w)\zeta_M(u) = \zeta_M(w * u)\,.$$

Exercise 7.

i) Prove Proposition 2.15, i.e. show that for $n \geq 1$ we have

$$4^n \zeta(\{3,1\}^n) = \zeta(\{4\}^n)\,.$$

ii) Show (2.7), i.e. show that we have for $n \geq 1$

$$\zeta(\{2\}^n) = \frac{\pi^{2n}}{(2n+1)!}\,.$$

(Hint: Calculate the coefficient of x^{2n} in (1.3).)

Exercise 8. Prove Proposition 2.25, i.e. show the following:

i) The space $\widetilde{\mathcal{M}}^{\mathbb{Q}}$ is closed under $q\frac{d}{dq}$.

ii) We have

$$\widetilde{\mathcal{M}}^{\mathbb{Q}} = \mathbb{Q}[\mathrm{g}(2), \mathrm{g}'(2), \mathrm{g}''(2)]\,.$$

where g' denotes the derivative with respect to $q\frac{d}{dq}$.

iii) Let $\mathbf{k} = (k_1, \dots, k_r)$ be an index with $k_1, \dots, k_r \geq 2$ even. Then we have

$$\mathrm{g}^{\mathrm{sym}}(\mathbf{k}) := \sum_{\sigma \in S_r} \mathrm{g}(k_{\sigma(1)}, \dots, k_{\sigma(r)}) \in \widetilde{\mathcal{M}}^{\mathbb{Q}}\,,$$

where S_r denotes the set of all permutations of $\{1, \dots, r\}$.

iv) We have

$$\widetilde{\mathcal{M}}^{\mathbb{Q}} = \left\langle \mathrm{g}^{\mathrm{sym}}(k_1, \dots, k_r) \;\middle|\; r \geq 0,\, k_1 \geq k_2 \geq \cdots \geq k_r \geq 2 \text{ even} \right\rangle_{\mathbb{Q}}\,,$$

where we set $\mathrm{g}^{\mathrm{sym}}(\emptyset) = 1$.

Exercise 9. Let $\bullet \in \{\sqcup\!\sqcup, *\}$.

i) Calculate $\zeta^{\bullet}(1,2,1)$.

ii) Show that

$$\zeta^{\bullet}(z_2 \sqcup\!\sqcup z_1 z_1 - z_2 * z_1 z_1) = 0\,,$$

by using the finite double shuffle relations and/or the duality relation and/or Eulers formula.

Exercise 10.

i) Show that for any admissible index $\mathbf{k}$ we have $\mathrm{ds}(z_1, z_{\mathbf{k}}) = z_1 ⧢ z_{\mathbf{k}} - z_1 * z_{\mathbf{k}} \in \mathfrak{H}^0$.

ii) Prove Hoffman's relation (Proposition 3.5) by using the extended double shuffle relations.

Exercise 11.

i) Show that $z_{\mathbf{k}^\dagger} = \tau(z_{\mathbf{k}})$ for any admissible index $\mathbf{k}$.

ii) Give the proof of Proposition 3.17.

Exercise 12.

i) Prove for $m \geq 1$ Euler's formula (4.21)

$$\mathsf{Z}(2m) = -\frac{B_{2m}}{2(2m)!}\left(-24\mathsf{Z}(2)\right)^m ,$$

by assuming the condition in i) of Theorem 4.17.

ii*) Assume the conditions in ii) of Theorem 4.17 hold. Try to find an explicit formula for $\mathsf{Z}(2m)$ as a polynomial in $\partial^j\,\mathsf{Z}(2)$ for $j \geq 0$, which generalizes Euler's formula

(Part ii) is a bonus exercise.)

Exercise 13. Show that the pairing $\langle\cdot,\cdot\rangle$ defined in (4.13) is Γ-invariant, bilinear, symmetric and non-degenerated. (i.e. prove Proposition 4.13).

Exercise 14.

i) Show that for a cusp form $f \in S_k$ and $\gamma \in \mathrm{SL}_2(\mathbb{Z})$ we have

$$(P_f \mid \gamma)(X,Y) = \int_{\gamma^{-1}(0)}^{\gamma^{-1}(i\infty)} (X - Y\tau)^{k-2} f(\tau)\, d\tau ,$$

where $\gamma(z) = \frac{az+b}{cz+d}$ for $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$.

ii) Use i) to show that for all $f \in S_k$ we have

$$P_f \mid (1+S) = P_f \mid (1+U+U^2) = 0 .$$

iii) Prove Lemma 4.27.

Exercise 15.

i) Let $p \in W_k^-$ and define $q = p \mid T$. Show that $A = H \mid (T' - 1)$, where $A = q^{od} - 3q^{ev}$ and $H = 2(q^{\mathrm{ev},+} - q^{\mathrm{od},+}) \in V_k^+$.

ii) Give the proof of Lemma 4.35 ii) by using i), i.e. show that in $\mathcal{D}_k$ the relation

$$\sum_{\substack{k_1+k_2=k \\ k_1,k_2\geq 1}} a_{k_1,k_2} P_{k_1,k_2} = \mu Z_k \,,$$

holds, if and only if $A = H \mid (1-S)$ for some polynomial $H \in V_k^U \cap V_k^+$. In this case we have

$$\mu = \langle H, \frac{X^{k-1} - Y^{k-1}}{X - Y} \rangle \,.$$

Here V_k^U denotes the space of U invariant polynomials, i.e. $H \,|\, U = H$.

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