

Relations satisfied by double q -zeta values

H. Bachmann, A. Burmester, U. Kühn

April 17, 2020

Abstract

We present recent results and conjectures for multiple q -zeta values. By that, we focus on our efforts to generalize the work of Gangl-Kaneko-Zagier to double q -zeta values.

Introduction

In this note we study the relations, which are satisfied by single and double q -zeta values. We start by recalling some aspects of multiple q -zeta values in section one. In section two we analyze distinct sets of relations and in the last section we study the interplay between those relations and the relations satisfied by single and double zeta values. We assume that the reader is familiar with the basic results for multiple zeta values and we use the notation as in [8].

Acknowledgements. The authors would like to thank Nils Matthes for his helpful comments and his contributions to this project. We also thank Hidekazu Furusho for making our participation at the RIMS Conference *Various Aspects of Multiple Zeta Values* (2019) possible. This project was partially supported by JSPS KAKENHI Grant 19K14499.

1 Multiple q -zeta values

Many of the most basic concepts in mathematics have so-called q -analogues, where q is a formal variable such that the specialization $q \rightarrow 1$ recovers the usual concept. In this report we will study the following q -analogues of multiple zeta values. If not stated otherwise, the results in this section are obtained in [6].

Definition 1.1. For integers $s_1, \dots, s_l \geq 1$ and $Q_1(t) \in t\mathbb{Q}[t]$ and $Q_2(t), \dots, Q_l(t) \in \mathbb{Q}[t]$ we call

$$\zeta_q(s_1, \dots, s_l; Q_1, \dots, Q_l) = \sum_{n_1 > \dots > n_l > 0} \frac{Q_1(q^{n_1})}{(1 - q^{n_1})^{s_1}} \cdots \frac{Q_l(q^{n_l})}{(1 - q^{n_l})^{s_l}} \in \mathbb{Q}[[q]]$$

a multiple q -zeta value.

The condition $Q_1(t) \in t\mathbb{Q}[t]$ assures $\zeta_q(s_1, \dots, s_l; Q_1, \dots, Q_l) \in \mathbb{Q}[[q]]$. Moreover, since we have for $s_1 > 1$

$$\lim_{q \rightarrow 1} (1 - q)^{s_1 + \dots + s_l} \zeta_q(s_1, \dots, s_l; Q_1, \dots, Q_l) = Q_1(1) \dots Q_l(1) \cdot \zeta(s_1, \dots, s_l),$$

such series indeed give q -analogues of multiple zeta values¹.

Definition 1.2. We set $\zeta_q(\emptyset; \emptyset) = 1$ and define the \mathbb{Q} -vector space of multiple q -zeta values to be

$$\mathcal{Z}_q := \left\langle \zeta_q(s_1, \dots, s_l; Q_1, \dots, Q_l) \mid l \geq 0, s_1, \dots, s_l \geq 1, \deg(Q_j) \leq s_j \right\rangle_{\mathbb{Q}}.$$

In fact \mathcal{Z}_q is a \mathbb{Q} -algebra, for example, it is

$$\zeta_q(s_1; Q_1) \cdot \zeta_q(s_2; Q_2) = \zeta_q(s_1, s_2; Q_1, Q_2) + \zeta_q(s_2, s_1; Q_2, Q_1) + \zeta_q(s_1 + s_2; Q_1 \cdot Q_2),$$

and clearly $\deg Q_1 \cdot Q_2 \leq s_1 + s_2$ if $\deg Q_j \leq s_j$ for $j = 1, 2$.

This model free approach to multiple q -zeta values recovers previously known multiple q -zeta values, where special choices for the $Q_i(t)$ have been made, e.g. the Bradley-Zhao model, the Schlesinger-Zudilin model and its extension by Ebrahimi-Fard-Manchon-Singer, the Okounkov-model and others, see e.g. [6], [13].

Remark 1.3. Caution: $s_1 + \dots + s_l$ does not give a good notion of weight for ζ_q . Also l will not be used to define the depth. Instead, we will consider a class of q -series which also spans the space \mathcal{Z}_q and use these series to define a weight and a depth filtration on \mathcal{Z}_q .

Definition 1.4. For natural numbers $s_1, \dots, s_l \geq 1$ and $r_1, \dots, r_l \geq 0$ the bi-brackets are defined by

$$\left(\begin{matrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{matrix} \right)_q = \kappa \cdot \sum_{n_1 > \dots > n_l > 0} \frac{n_1^{r_1} P_{s_1-1}(q^{n_1}) \dots n_l^{r_l} P_{s_l-1}(q^{n_l})}{(1 - q^{n_1})^{s_1} \dots (1 - q^{n_l})^{s_l}} \in \mathbb{Q}[[q]],$$

where $\kappa = (r_1!(s_1 - 1)! \dots r_l!(s_l - 1)!)^{-1}$ and the $P_{k-1}(t)$ are the Eulerian polynomials defined by

$$\frac{P_{k-1}(t)}{(1 - t)^k} = \text{Li}_{1-k}(t) = \sum_{d > 0} d^{k-1} t^d.$$

For example we have $P_0(t) = P_1(t) = t$ and $P_2(t) = t^2 + t$. If $r_1 = \dots = r_l = 0$, then bi-brackets specialize to the brackets defined in [5], i.e.,

$$\left(\begin{matrix} s_1, \dots, s_l \\ 0, \dots, 0 \end{matrix} \right)_q = \left(s_1, \dots, s_l \right)_q = \frac{1}{(s_1 - 1)! \dots (s_l - 1)!} \sum_{n > 0} \left(\sum_{\substack{u_1 v_1 + \dots + u_l v_l = n \\ u_1 > \dots > u_l > 0 \\ v_1, \dots, v_l > 0}} v_1^{s_1} \dots v_l^{s_l} \right) q^n.$$

In the case $l = 1$ we get the classical divisor sums $\sigma_{k-1}(n) = \sum_{d|n} d^{k-1}$ and the single brackets appear in the Fourier expansion of classical Eisenstein series, which are (quasi)-modular forms for $\text{SL}_2(\mathbb{Z})$, for example

$$G_2 = -\frac{1}{24} + \left(2 \right)_q, \quad G_4 = \frac{1}{1440} + \left(4 \right)_q, \quad G_6 = -\frac{1}{60480} + \left(6 \right)_q.$$

¹ We use the convention $\zeta(s_1, \dots, s_l) = \sum_{n_1 > \dots > n_l > 0} \frac{1}{n_1^{s_1} \dots n_l^{s_l}}$.

Theorem 1.5. The following equality holds

$$\mathcal{Z}_q = \left\langle \left(\begin{array}{c} s_1, \dots, s_l \\ r_1, \dots, r_l \end{array} \right)_q \mid l \geq 0, s_1, \dots, s_l \geq 1, r_1, \dots, r_l \geq 0 \right\rangle_{\mathbb{Q}}.$$

The main idea of proof is illustrated by the following example

$$\begin{aligned} \left(\begin{array}{c} 1, 1 \\ 0, 1 \end{array} \right)_q &= \sum_{n_1 > n_2 > 0} \frac{q^{n_1}}{(1 - q^{n_1})} \frac{n_2 q^{n_2}}{(1 - q^{n_2})} \\ &= \sum_{n_1 > n_2 > 0} \frac{q^{n_1}}{(1 - q^{n_1})} \frac{q^{n_2}}{(1 - q^{n_2})} + \sum_{n_1 > n_2 > n_3 > 0} \frac{q^{n_1}}{(1 - q^{n_1})} \frac{q^{n_2}}{(1 - q^{n_2})} \frac{1 - q^{n_3}}{(1 - q^{n_3})} \\ &= \zeta_q(1, 1; t, t) + \zeta_q(1, 1, 1; t, t, 1 - t). \end{aligned}$$

Remark 1.6. (i) The (bi)-brackets have also a direct connection to multiple zeta values, since if $s_1 > r_1 + 1$ and $s_j \geq r_j + 1$ for $j = 2, \dots, l$, then

$$\lim_{q \rightarrow 1} (1 - q)^{s_1 + \dots + s_l} \left(\begin{array}{c} s_1, \dots, s_l \\ r_1, \dots, r_l \end{array} \right)_q = \frac{1}{r_1! \cdot \dots \cdot r_l!} \zeta(s_1 - r_1, \dots, s_l - r_l). \quad (1.1)$$

(ii) Another very interesting connection to multiple zeta values is given by the Fourier expansion of multiple Eisenstein series, for more details we refer to [1], [7].

Definition 1.7. We endow the space of multiple q -zeta values \mathcal{Z}_q with the weight-filtration Fil^W resp. depth-filtration Fil^D induced by the notion of weight and depth defined on the bi-brackets, namely the sum of all the indices s_i and r_i and the number l .

Conjecture 1.8. We conjecture the following refinements of Theorem 1.5.

(B0)

$$\mathcal{Z}_q = \left\langle \left(\begin{array}{c} s_1, \dots, s_l \\ r_1, \dots, r_l \end{array} \right)_q \mid \begin{array}{l} l \geq 0 \\ s_i > r_i \text{ for all } i = 1, \dots, l \\ s_i + r_i \text{ odd, if } l - i \text{ odd} \end{array} \right\rangle_{\mathbb{Q}}$$

and this spanning set respects the weight and depth filtration given in Definition 1.7.

(B1) Multiple q -zeta values are linear combinations of brackets.

(B2) Multiple q -zeta values are linear combinations of "123"-brackets, i.e.

$$\mathcal{Z}_q = \left\langle \left(s_1, \dots, s_l \right)_q \mid s_i \in \{1, 2, 3\} \text{ for all } i = 1, \dots, l \right\rangle_{\mathbb{Q}}.$$

In contrast to the case of multiple zeta values, where it is expected that $\zeta(s_1, \dots, s_l)$ with $s_i \in \{2, 3\}$ form basis, we have relations among the brackets in (B2) starting in weight 6. Given the alphabet $A_z = \{z_{s,r} \mid s \geq 1, r \geq 0\}$ we define the quasi-shuffle product \diamond on $\mathbb{Q}\langle A_z \rangle$ recursively. Let $u, v \in A_z^*$ be words, then $1 \diamond u = u \diamond 1 = u$ and

$$z_{s_1, r_1} u \diamond z_{s_2, r_2} v = z_{s_1, r_1} (u \diamond z_{s_2, r_2} v) + z_{s_2, r_2} (z_{s_1, r_1} u \diamond v) + (z_{s_2, r_2} \circ z_{s_1, r_1}) (u \diamond v),$$

where

$$z_{s_2, r_2} \circ z_{s_1, r_1} = \binom{r_1 + r_2}{r_2} \left(z_{s_1 + s_2, r_1 + r_2} + \sum_{j=1}^{s_1} \lambda_{s_1, s_2}^j z_{j, r_1 + r_2} + \sum_{j=1}^{s_2} \lambda_{s_2, s_1}^j z_{j, r_1 + r_2} \right)$$

and with the Bernoulli numbers B_n we have

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

Furthermore, we let²

$$\mathcal{A} \left(\begin{matrix} X_1, X_2, \dots, X_l \\ Y_1, Y_2, \dots, Y_l \end{matrix} \right) = \sum_{\substack{s_1, \dots, s_l \geq 1 \\ r_1, \dots, r_l \geq 0}} z_{s_1, r_1} \dots z_{s_l, r_l} X_1^{s_1-1} \dots X_l^{s_l-1} Y_1^{r_1} \dots Y_l^{r_l}$$

be the generating series of words of depth l . Then for each l we set

$$\tau \left(\mathcal{A} \left(\begin{matrix} X_1, X_2, \dots, X_l \\ Y_1, Y_2, \dots, Y_l \end{matrix} \right) \right) = \mathcal{A} \left(\begin{matrix} Y_1 + \dots + Y_l, \dots, Y_1 + Y_2, Y_1 \\ X_l, X_{l-1} - X_l, \dots, X_1 - X_2 \end{matrix} \right)$$

and define the involution τ on $\mathbb{Q}\langle A_z \rangle$ by setting

$$\tau(z_{s_1, r_1} \dots z_{s_l, r_l}) = \text{coefficient of } X_1^{s_1-1} \dots X_l^{s_l-1} Y_1^{r_1} \dots Y_l^{r_l} \text{ in } \tau \left(\mathcal{A} \left(\begin{matrix} X_1, X_2, \dots, X_l \\ Y_1, Y_2, \dots, Y_l \end{matrix} \right) \right).$$

Theorem 1.9 ([1],[2]). The vector space of bi-brackets is a \mathbb{Q} -algebra with derivation $q \frac{d}{dq}$. More precisely, the map $(\mathbb{Q}\langle A_z \rangle, \diamond) \rightarrow \mathcal{Z}_q$ given by $z_{s_1, r_1} \dots z_{s_l, r_l} \mapsto \left(\begin{matrix} s_1, \dots, s_l \\ r_1, \dots, r_l \end{matrix} \right)_q$ is a τ -invariant algebra homomorphism.

A key ingredient for the proof is to relate the product \diamond to certain functional equations of the generating series of bi-brackets and then to check those by using the following explicit description

$$\begin{aligned} \mathfrak{g} \left(\begin{matrix} X_1, \dots, X_l \\ Y_1, \dots, Y_l \end{matrix} \right) &= \sum_{\substack{s_1, \dots, s_l \geq 1 \\ r_1, \dots, r_l \geq 0}} \binom{s_1, \dots, s_l}{r_1, \dots, r_l}_q X_1^{s_1-1} \dots X_l^{s_l-1} Y_1^{r_1} \dots Y_l^{r_l} \\ &= \sum_{m_1 > \dots > m_l > 0} \prod_{j=1}^l e^{m_j Y_j} \frac{e^{X_j} q^{m_j}}{1 - e^{X_j} q^{m_j}} \in \mathbb{Q}[[q]][[X_1, Y_1, \dots, X_l, Y_l]]. \end{aligned}$$

A big quest in the history of multiple q -zeta values had been the search for a model that is dimorphic and compatible to multiple zeta values, i.e. it satisfies a stuffle and a shuffle formula for the product, which specialize via $q \rightarrow 1$ to the classical double shuffle, see e.g. [13]. This is the case for the bi-brackets by employing the identity $a \cdot b = \tau(\tau(a) \cdot \tau(b))$. However, a disadvantage of the bi-brackets is that their product is only filtered and not graded with respect to the weight.

We define now the q -stuffle product $*$ on $\mathbb{Q}\langle A_z \rangle$ recursively. Let $u, v \in A_z^*$ be words, then $1 * u = u * 1 = u$ and

$$z_{s_1, r_1} u * z_{s_2, r_2} v = z_{s_1, r_1} (u * z_{s_2, r_2} v) + z_{s_2, r_2} (z_{s_1, r_1} u * v) + \binom{r_1 + r_2}{r_2} z_{s_1 + s_2, r_1 + r_2} (u * v).$$

We observe that $*$ respects the natural weight grading on $\mathbb{Q}\langle A_z \rangle$ given by the sum of all indices s_i and r_i .

²More precisely, we denote by \mathcal{A} the bimould of generating series for A_z^* ordered by depth, i.e. we have a sequence $\mathcal{A} = \left(\mathcal{A} \left(\begin{matrix} X \\ Y \end{matrix} \right), \mathcal{A} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right), \dots \right)$ and it is clear by the number of variables which element we have to take.

Definition 1.10. We define the algebra \mathcal{Z}_q^f of formal multiple q -zeta values to be the graded algebra with the universal property that any τ -invariant algebra homomorphism $(\mathbb{Q}\langle A_z \rangle, *) \rightarrow A$ factors through \mathcal{Z}_q^f , i.e. we require a commutative diagramm

$$\begin{array}{ccc} (\mathbb{Q}\langle A_z \rangle, *) & \longrightarrow & \mathcal{Z}_q^f \\ & \searrow & \downarrow \text{Y} \\ & & A \end{array}$$

Remark 1.11. (i) One could construct \mathcal{Z}_q^f as the polynomial ring in formal variables $\zeta_q^f(s_1, \dots, s_l)$ modulo the relations given by the requirements that the bimould given by the generating series of these variables is symmetril and swap-invariant. For the reader we explain these notations in an example. Let $\mathcal{Z} = \left(\mathcal{Z} \binom{X}{Y}, \mathcal{Z} \binom{X_1, X_2}{Y_1, Y_2} \right)$ be the bimould given by

$$\mathcal{Z} \binom{X}{Y} = \sum_{\substack{s \geq 1 \\ r \geq 0}} \zeta_q^f(s) X^{s-1} Y^r, \quad \mathcal{Z} \binom{X_1, X_2}{Y_1, Y_2} = \sum_{\substack{s_1, s_2 \geq 1 \\ r_1, r_2 \geq 0}} \zeta_q^f(s_1, s_2) X_1^{s_1-1} X_2^{s_2-1} Y_1^{r_1} Y_2^{r_2}.$$

Then \mathcal{Z} is swap-invariant if and only if

$$\mathcal{Z} \binom{X_1}{Y_1} = \mathcal{Z} \binom{Y_1}{X_1}, \quad \mathcal{Z} \binom{X_1, X_2}{Y_1, Y_2} = \mathcal{Z} \binom{Y_1 + Y_2, Y_1}{X_2, X_1 - X_2} \quad (1.2)$$

and \mathcal{Z} is symmetril if and only if

$$\mathcal{Z} \binom{X_1}{Y_1} \mathcal{Z} \binom{X_2}{Y_2} = \mathcal{Z} \binom{X_1, X_2}{Y_1, Y_2} + \mathcal{Z} \binom{X_2, X_1}{Y_2, Y_1} + \frac{1}{X_1 - X_2} \left(\mathcal{Z} \binom{X_1}{Y_1 + Y_2} - \mathcal{Z} \binom{X_2}{Y_1 + Y_2} \right). \quad (1.3)$$

For more details on moulds and bimoulds we refer to [11].

(ii) The map $\partial : \mathcal{Z}_q^f \rightarrow \mathcal{Z}_q^f$ given by $\partial \zeta_q^f(s_1, \dots, s_l) = \sum_{i=1}^l s_i (r_i + 1) \zeta_q^f(s_1, \dots, s_i + 1, \dots, s_l)$ is a derivation.

For the algebra structure of \mathcal{Z}_q , we conjecture the following.

Conjecture 1.12. The algebra \mathcal{Z}_q is a graded and there is an isomorphism of graded algebras $\mathcal{Z}_q^f \rightarrow \mathcal{Z}_q$.

Using the description of \mathcal{Z}_q^f in the language of bimoulds, see Remark (1.11) (i), we have the following evidence towards Conjecture 1.12.

Theorem 1.13 ([4] and [3]). There are formal power series

$$\mathcal{G} \binom{X}{Y} = \sum_{\substack{s \geq 1 \\ r \geq 0}} G \binom{s}{r} X^{s-1} Y^r \in \mathcal{Z}_q[[X, Y]], \quad (1.4)$$

$$\mathcal{G} \binom{X_1, X_2}{Y_1, Y_2} = \sum_{\substack{s_1, s_2 \geq 1 \\ r_1, r_2 \geq 0}} G \binom{s_1, s_2}{r_1, r_2} X_1^{s_1-1} X_2^{s_2-1} Y_1^{r_1} Y_2^{r_2} \in \mathcal{Z}_q[[X_1, Y_1, X_2, Y_2]], \quad (1.5)$$

$$\mathcal{G} \binom{X_1, X_2, X_3}{Y_1, Y_2, Y_3} = \sum_{\substack{s_1, s_2, s_3 \geq 1 \\ r_1, r_2, r_3 \geq 0}} G \binom{s_1, s_2, s_3}{r_1, r_2, r_3} X_1^{s_1-1} X_2^{s_2-1} X_3^{s_3-1} Y_1^{r_1} Y_2^{r_2} Y_3^{r_3} \in \mathcal{Z}_q[[X_1, Y_1, X_2, Y_2, X_3, Y_3]], \quad (1.6)$$

such that the bimould $\mathcal{G} = \left(\mathcal{G} \binom{X}{Y}, \mathcal{G} \binom{X_1, X_2}{Y_1, Y_2}, \mathcal{G} \binom{X_1, X_2, X_3}{Y_1, Y_2, Y_3} \right)$ is symmetril and swap-invariant and such that the coefficients of (1.4), (1.5) and (1.6) successively span

$$\text{Fil}_1^D(\mathcal{Z}_q) \subseteq \text{Fil}_2^D(\mathcal{Z}_q) \subseteq \text{Fil}_3^D(\mathcal{Z}_q).$$

Observe, according to Conjecture 1.12 the map $\mathcal{Z}_q^f \rightarrow \mathcal{Z}_q$ given by $\zeta_q^f \binom{s_1, \dots, s_l}{r_1, \dots, r_l} \mapsto G \binom{s_1, \dots, s_l}{r_1, \dots, r_l}$ for $l = 1, 2$ and 3 should have an extension to all depths. Below we sketch the proof for depth up to 2 only. The method to establish the depth 3 case is slightly more conceptual and probably extends to higher depth [3].

Idea of Proof: First we prove the existence of a symmetril and swap-invariant bimould $\tilde{\beta} = \left(\tilde{\beta} \binom{X}{Y}, \tilde{\beta} \binom{X_1, X_2}{Y_1, Y_2} \right)$, where

$$\tilde{\beta} \binom{X}{Y} = - \sum_{k \geq 2} \frac{B_k}{2k!} X^{k-1} - \sum_{k \geq 2} \frac{B_k}{2k!} Y^{k-1}$$

and the power series $\tilde{\beta} \binom{X_1, X_2}{Y_1, Y_2}$ is made out of a Bernoulli realisation for double zeta values, see Remark 3.4. We set

$$\begin{aligned} \mathcal{G} \binom{X}{Y} &= \tilde{\beta} \binom{X}{Y} + \mathfrak{g} \binom{X}{Y}, & (1.7) \\ \mathcal{G} \binom{X_1, X_2}{Y_1, Y_2} &= \tilde{\beta} \binom{X_1, X_2}{Y_1, Y_2} + \tilde{\beta} \binom{X_2}{Y_2} \mathfrak{g} \binom{X_1}{Y_1} + \tilde{\beta} \binom{X_1 - X_2}{Y_1} \mathfrak{g} \binom{X_2}{Y_1 + Y_2} \\ &\quad - \tilde{\beta} \binom{X_1 - X_2}{Y_2} \mathfrak{g} \binom{X_1}{Y_1 + Y_2} - \frac{1}{2} \mathfrak{g} \binom{X_1}{Y_1 + Y_2} + \mathfrak{g} \binom{X_1, X_2}{Y_1, Y_2}. & (1.8) \end{aligned}$$

Then, using the functional equations for the generating series of bi-brackets, we check swap-invariance and symmetrility. Now the claim follows, since by Theorem 1.5 the coefficients of (1.7) span $\text{Fil}_1^D(\mathcal{Z}_q)$ and those of (1.7) and (1.8) span $\text{Fil}_2^D(\mathcal{Z}_q)$. \square

Definition 1.14. The coefficients of (1.4), (1.5) and (1.6) are called combinatorial multiple Eisenstein series.

Remark 1.15. (i) This notation is due to the fact that combinatorial multiple Eisenstein series of depth one are given by classical Eisenstein series and their derivatives, whenever $s + r$ is even. Moreover, similar linear combinations of bi-brackets occur in the Fourier expansion of multiple Eisenstein series, see [9], [2], [7].

(ii) The combinatorial multiple Eisenstein series satisfy the algebraic double q-shuffle relations (see Definition 2.2), namely

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

and taking the limit $q \rightarrow 1$ similar to (1.1) yields the algebraic double shuffle relations for multiple zeta values (see Definition 3.2).

(iii) In addition we have

$$q \frac{d}{dq} \mathcal{G}_1 \left(\begin{matrix} X \\ Y \end{matrix} \right) = \frac{\partial^2}{\partial X \partial Y} \mathcal{G}_1 \left(\begin{matrix} X \\ Y \end{matrix} \right), \quad \text{and} \quad q \frac{d}{dq} \mathcal{G}_2 \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right) = \left(\frac{\partial^2}{\partial X_1 \partial Y_1} + \frac{\partial^2}{\partial X_2 \partial Y_2} \right) \mathcal{G}_2 \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right)$$

2 Relations satisfied by double q -zeta values

If not stated otherwise, the results in this section are obtained in [4].

Notation 2.1. Let A be a \mathbb{Q} -algebra. In the following $\mathcal{Z} = \left(\mathcal{Z} \left(\begin{matrix} X \\ Y \end{matrix} \right), \mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right) \right)$ denotes a bimould of formal power series

$$\begin{aligned} \mathcal{Z} \left(\begin{matrix} X \\ Y \end{matrix} \right) &= \sum_{\substack{s \geq 1 \\ r \geq 0}} Z \binom{s}{r} X^{s-1} Y^r \in A[[X, Y]], \\ \mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right) &= \sum_{\substack{s_1, s_2 \geq 1 \\ r_1, r_2 \geq 0}} Z \binom{s_1, s_2}{r_1, r_2} X_1^{s_1-1} X_2^{s_2-1} Y_1^{r_1} Y_2^{r_2} \in A[[X_1, X_2, Y_1, Y_2]]. \end{aligned}$$

Definition 2.2. Let $\mathcal{Z} = \left(\mathcal{Z} \left(\begin{matrix} X \\ Y \end{matrix} \right), \mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right) \right)$ be a bimould.

(a) We say \mathcal{Z} satisfies the algebraic double q -shuffle relations, if

$$\begin{aligned} \mathcal{Z} \left(\begin{matrix} X_1 \\ Y_1 \end{matrix} \right) \mathcal{Z} \left(\begin{matrix} X_2 \\ Y_2 \end{matrix} \right) &= \mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right) + \mathcal{Z} \left(\begin{matrix} X_2, X_1 \\ Y_2, Y_1 \end{matrix} \right) + \frac{1}{X_1 - X_2} \left(\mathcal{Z} \left(\begin{matrix} X_1 \\ Y_1 + Y_2 \end{matrix} \right) - \mathcal{Z} \left(\begin{matrix} X_2 \\ Y_1 + Y_2 \end{matrix} \right) \right) \\ &= \mathcal{Z} \left(\begin{matrix} X_1 + X_2, X_1 \\ Y_2, Y_1 - Y_2 \end{matrix} \right) + \mathcal{Z} \left(\begin{matrix} X_1 + X_2, X_2 \\ Y_1, Y_2 - Y_1 \end{matrix} \right) + \frac{1}{Y_1 - Y_2} \left(\mathcal{Z} \left(\begin{matrix} X_1 + X_2 \\ Y_1 \end{matrix} \right) - \mathcal{Z} \left(\begin{matrix} X_1 + X_2 \\ Y_2 \end{matrix} \right) \right). \end{aligned} \quad (2.1)$$

(b) We say \mathcal{Z} satisfies the linear double q -shuffle relation, if $\mathcal{Z} \left(\begin{matrix} X \\ Y \end{matrix} \right)$ and $\mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right)$ solves the equation

$$\begin{aligned} &\mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right) + \mathcal{Z} \left(\begin{matrix} X_2, X_1 \\ Y_2, Y_1 \end{matrix} \right) + \frac{1}{X_1 - X_2} \left(\mathcal{Z} \left(\begin{matrix} X_1 \\ Y_1 + Y_2 \end{matrix} \right) - \mathcal{Z} \left(\begin{matrix} X_2 \\ Y_1 + Y_2 \end{matrix} \right) \right) \\ &- \mathcal{Z} \left(\begin{matrix} X_1 + X_2, X_1 \\ Y_2, Y_1 - Y_2 \end{matrix} \right) - \mathcal{Z} \left(\begin{matrix} X_1 + X_2, X_2 \\ Y_1, Y_2 - Y_1 \end{matrix} \right) - \frac{1}{Y_1 - Y_2} \left(\mathcal{Z} \left(\begin{matrix} X_1 + X_2 \\ Y_1 \end{matrix} \right) - \mathcal{Z} \left(\begin{matrix} X_1 + X_2 \\ Y_2 \end{matrix} \right) \right) = 0. \end{aligned} \quad (2.2)$$

Remark 2.3. (i) Of course, (a) implies (b).

(ii) If $\mathcal{Z} = \left(\mathcal{Z} \left(\begin{matrix} X \\ Y \end{matrix} \right), \mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right) \right)$ is a symmetril and swap-invariant bimould, then it satisfies the algebraic double q -shuffle relations. Since (2.1) is nothing else than the expansion of the equality

$$\mathcal{Z} \left(\begin{matrix} X_1 \\ Y_1 \end{matrix} \right) \mathcal{Z} \left(\begin{matrix} X_2 \\ Y_2 \end{matrix} \right) = \tau \left(\tau \left(\mathcal{Z} \left(\begin{matrix} X_1 \\ Y_1 \end{matrix} \right) \right) \tau \left(\mathcal{Z} \left(\begin{matrix} X_2 \\ Y_2 \end{matrix} \right) \right) \right)$$

by means of the formula (1.3).

(iii) If $\mathcal{Z} = \left(\mathcal{Z} \left(\begin{matrix} X \\ Y \end{matrix} \right), \mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right) \right)$ is a symmetril and swap-invariant bimould, then beside of (1.2) and (2.2) there are the linear relations inbetween the coefficients of $\mathcal{Z} \left(\begin{matrix} X \\ Y \end{matrix} \right)$ and $\mathcal{Z} \left(\begin{matrix} X_1, X_2 \\ Y_1, Y_2 \end{matrix} \right)$ given by expanding the equality

$$\mathcal{Z} \left(\begin{matrix} X_1 \\ Y_1 \end{matrix} \right) \mathcal{Z} \left(\begin{matrix} X_2 \\ Y_2 \end{matrix} \right) = \mathcal{Z} \left(\begin{matrix} X_1 \\ Y_1 \end{matrix} \right) \mathcal{Z} \left(\begin{matrix} Y_2 \\ X_2 \end{matrix} \right).$$

Proposition 2.4. Assume $\mathcal{Z} = \left(\mathcal{Z} \begin{pmatrix} X \\ Y \end{pmatrix}, \mathcal{Z} \begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} \right)$ satisfies the linear double q -shuffle relation.

(a) We have

$$Z \begin{pmatrix} 2 \\ 0 \end{pmatrix} = Z \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad Z \begin{pmatrix} 8 \\ 0 \end{pmatrix} = 12 Z \begin{pmatrix} 4, 4 \\ 0, 0 \end{pmatrix}. \quad (2.3)$$

(b) For even $k \geq 4$ we have the identities

$$\sum_{\substack{s_1+s_2=k \\ s_1, s_2 \text{ even}}} Z \begin{pmatrix} s_1, s_2 \\ 0, 0 \end{pmatrix} = \frac{3}{4} Z \begin{pmatrix} k \\ 0 \end{pmatrix} - \frac{1}{2} Z \begin{pmatrix} k-1 \\ 1 \end{pmatrix}, \quad (2.4)$$

$$\sum_{\substack{s_1+s_2=k \\ s_1 > 1, s_2 \text{ odd}}} Z \begin{pmatrix} s_1, s_2 \\ 0, 0 \end{pmatrix} = \frac{1}{4} Z \begin{pmatrix} k \\ 0 \end{pmatrix} - \frac{1}{2} Z \begin{pmatrix} k-1 \\ 1 \end{pmatrix}. \quad (2.5)$$

Proof. Let p_k be homogenous polynomials of degree $k - 2$ such that

$$\begin{aligned} \sum_{k=2}^{\infty} p_k(X_1, X_2, Y_1, Y_2) &= \mathcal{Z} \begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} + \mathcal{Z} \begin{pmatrix} X_2, X_1 \\ Y_2, Y_1 \end{pmatrix} + \frac{1}{X_1 - X_2} \left(\mathcal{Z} \begin{pmatrix} X_1 \\ Y_1 + Y_2 \end{pmatrix} - \mathcal{Z} \begin{pmatrix} X_2 \\ Y_1 + Y_2 \end{pmatrix} \right) \\ &\quad - \mathcal{Z} \begin{pmatrix} X_1 + X_2, X_1 \\ Y_2, Y_1 - Y_2 \end{pmatrix} - \mathcal{Z} \begin{pmatrix} X_1 + X_2, X_2 \\ Y_1, Y_2 - Y_1 \end{pmatrix} - \frac{1}{Y_1 - Y_2} \left(\mathcal{Z} \begin{pmatrix} X_1 + X_2 \\ Y_1 \end{pmatrix} - \mathcal{Z} \begin{pmatrix} X_1 + X_2 \\ Y_2 \end{pmatrix} \right). \end{aligned}$$

Let $c_{p_k}(X_1^a X_2^b)$ denote the coefficient of $X_1^a X_2^b$ in p_k , which must be zero by (2.2). Then the first identity of (a) is given by $Z \begin{pmatrix} 2 \\ 0 \end{pmatrix} - Z \begin{pmatrix} 1 \\ 1 \end{pmatrix} = c_{p_2}(1) = 0$ and the second by

$$12 Z \begin{pmatrix} 4, 4 \\ 0, 0 \end{pmatrix} - Z \begin{pmatrix} 8 \\ 0 \end{pmatrix} = 2c_{p_8}(X_1^2 X_2^4) - 3c_{p_8}(X_1^3 X_2^3) + 2c_{p_8}(X_1^4 X_2^2) = 0.$$

The identities in (b) are given by the equalities

$$\frac{1}{2} p_k(1, 0, 0, 0) \pm \frac{1}{4} p_k(1, -1, 0, 0) = 0.$$

□

Theorem 2.5. Assume $\mathcal{Z} = \left(\mathcal{Z} \begin{pmatrix} X \\ Y \end{pmatrix}, \mathcal{Z} \begin{pmatrix} X_1, X_2 \\ Y_1, Y_2 \end{pmatrix} \right)$ satisfies the algebraic double q -shuffle relations, $Z \begin{pmatrix} 2 \\ 0 \end{pmatrix} \neq 0$ and ∂ is a derivation on A s.t. $\partial Z \begin{pmatrix} s \\ r \end{pmatrix} = s(r+1)Z \begin{pmatrix} s+1 \\ r+1 \end{pmatrix}$. Then

$$\partial^3 Z \begin{pmatrix} 2 \\ 0 \end{pmatrix} + 24 Z \begin{pmatrix} 2 \\ 0 \end{pmatrix} \partial^2 Z \begin{pmatrix} 2 \\ 0 \end{pmatrix} - 36 (\partial Z \begin{pmatrix} 2 \\ 0 \end{pmatrix})^2 = 0 \quad (2.6)$$

and if $r + s$ is even, then there exists a homogenous polynomial $g_{r,s} \in \mathbb{Q}[t_1, t_2, t_3]$ such that

$$Z \begin{pmatrix} s \\ r \end{pmatrix} = g_{r,s} \left(Z \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \partial Z \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \partial^2 Z \begin{pmatrix} 2 \\ 0 \end{pmatrix} \right).$$

Idea of proof: We express (2.4) in terms of products, i.e.

$$\sum_{i=1}^{k/2-1} Z \begin{pmatrix} 2i \\ 0 \end{pmatrix} Z \begin{pmatrix} k-2i \\ 0 \end{pmatrix} = \frac{k+1}{2} Z \begin{pmatrix} k \\ 0 \end{pmatrix} - Z \begin{pmatrix} k-1 \\ 1 \end{pmatrix}.$$

Since in addition $Z \begin{pmatrix} k-1 \\ 1 \end{pmatrix} = \frac{1}{k-2} \partial Z \begin{pmatrix} k-2 \\ 0 \end{pmatrix}$, we get recursion for $Z \begin{pmatrix} k \\ 0 \end{pmatrix}$ in terms of the $Z \begin{pmatrix} 2 \\ 0 \end{pmatrix}$ and its derivatives. The formula $Z \begin{pmatrix} 8 \\ 0 \end{pmatrix} = 12 Z \begin{pmatrix} 4, 4 \\ 0, 0 \end{pmatrix}$ of Proposition 2.4 gives the further expression $Z \begin{pmatrix} 8 \\ 0 \end{pmatrix} = \frac{6}{7} Z \begin{pmatrix} 4 \\ 0 \end{pmatrix}^2$, which in turn leads to the claimed differential equation. □

Remark 2.6. (i) The space of solutions for (2.6) is small, therefore there are not many choices for $Z\binom{2}{0}$ in general.

(ii) The above theorem gives an alternative proof of the fact that the ring of quasi-modular form is generated by G_2 , $G'_2 := q\frac{d}{dq}G_2$ and $G''_2 := \left(q\frac{d}{dq}\right)^2G_2$.

(iii) A detailed study of the recursion gives

$$Z\binom{2k}{0} = (-1)^{k-1} \frac{B_{2k}}{2(2k)!} \left(24 Z\binom{2}{0}\right)^k + \text{more terms which contain } \partial \quad (2.7)$$

Definition 2.7. Let k be even, then we refer to homogenous polynomials $p \in \mathbb{Q}[X_1, X_2, Y_1, Y_2]$ of degree $k - 2$ and of the form

$$\begin{aligned} p(X_1, X_2, Y_1, Y_2) &= p(-X_1, X_2, -Y_1, Y_2) = -p(X_2, X_1, Y_2, Y_1) \\ p(X_1, X_2, Y_1, Y_2) - p(X_1 + X_2, X_2, Y_1, Y_2 - Y_1) - p(X_1, X_1 + X_2, Y_1 - Y_2, Y_2) &= 0, \end{aligned}$$

as the odd q -period polynomial for $\text{SL}_2(\mathbb{Z})$ of weight k .

Theorem 2.8. Let k be even. Assume $\mathcal{Z} = \left(\mathcal{Z}\binom{X}{Y}, \mathcal{Z}\binom{X_1, X_2}{Y_1, Y_2}\right)$ satisfies the linear double q -shuffle relation, then each odd q -period polynomial for $\text{SL}_2(\mathbb{Z})$ of weight k determines a \mathbb{Q} -linear relations of the form

$$\sum_{\substack{r_1+r_2+s_1+s_2=k \\ r_1+s_1 \text{ odd}}} \lambda_{r_1, r_2}^{s_1, s_2} Z\binom{s_1, s_2}{r_1, r_2} = \sum_{\substack{u_1+u_2+v_1+v_2=k \\ u_1+v_1 \text{ even}}} \mu_{v_1, v_2}^{u_1, u_2} \left(Z\binom{u_1, u_2}{v_1, v_2} + Z\binom{u_2, u_1}{v_2, v_1} \right) + \sum_{u+v=k} \mu_{u, v} Z\binom{u}{v}. \quad (2.8)$$

More precisely, the rational numbers $\lambda_{r_1, r_2}^{s_1, s_2}$, $\mu_{v_1, v_2}^{u_1, u_2}$ and $\mu_{u, v}$ can be explicitly calculated from the coefficients of the q -period polynomial.

Remark 2.9. (i) The relations (2.8) will be called exotic relations.

(ii) If the bimould \mathcal{Z} satisfies beside the linear double q -shuffle relation no other linear relations in weight k , then the vector space of exotic relations actually corresponds to the vector space of the odd q -period polynomials of weight k .

(iii) For example we get in weight 12

$$\begin{aligned} 28 Z\binom{9,3}{0,0} + 150 Z\binom{7,5}{0,0} + 168 Z\binom{5,7}{0,0} \\ = 28 \left(Z\binom{8,4}{0,0} + Z\binom{4,8}{0,0} \right) + \frac{190}{3} Z\binom{6,6}{0,0} + 4 Z\binom{12}{0}. \end{aligned} \quad (2.9)$$

(iv) Of course, the combinatorial multiple Eisenstein series satisfy (2.9) and in that cases the right hand side equals a modular form. Note that similar expressions have been obtained also by Tasaka [12]. Now taking the limit $q \rightarrow 1$ as in (1.1) yields the famous relation of Gangl-Kaneko-Zagier, [9] Example 2.

Theorem 2.10. Assume $\mathcal{Z} = \left(\mathcal{Z} \binom{X}{Y}, \mathcal{Z} \binom{X_1, X_2}{Y_1, Y_2} \right)$ satisfies the algebraic double q -shuffle relations, then

$$F \binom{X}{Y} = \frac{1}{X} + \frac{1}{Y} + \mathcal{Z} \binom{-X}{-Y} - \mathcal{Z} \binom{X}{Y}$$

satisfies the Fay identity

$$F \binom{X_1}{Y_1} F \binom{X_2}{Y_2} + F \binom{X_1 - X_2}{-Y_2} F \binom{X_1}{Y_1 + Y_2} + F \binom{-X_2}{-Y_1 - Y_2} F \binom{X_1 - X_2}{Y_1} = 0.$$

Idea of proof: We use for the product $F \binom{X_1}{Y_1} F \binom{X_2}{Y_2}$ the shuffle product formula to evaluate the products where both factors have the same inside sign and the stuffle formula for those where the inside signs are different. Then we proceed in a similar vein for the remaining terms. Finally one can check after an easy but tedious calculation that all these long expressions sum up to zero. \square

Remark 2.11. (i) In [4] we show that any odd power series $\mathcal{Z} \in A[[X, Y]]$, for which the Laurent series

$$F \binom{X}{Y} = -\frac{1}{2} \left(\frac{1}{X} + \frac{1}{Y} \right) + \mathcal{Z} \binom{X}{Y}$$

satisfies the Fay identity (see e.g. [10]), gives an (explicit) solution to the double q -shuffle relation.

(ii) In [9], Theorem 4, similar results are proven for the double zeta values. In analogy we could view the homogenous parts of $F \binom{X_1}{Y_1} F \binom{X_2}{Y_2}$ as extended q -period polynomials.

Conjecture 2.12. Let \mathcal{D} be the \mathbb{Q} -vector space spanned by the formal variables

$$\left\{ Z \binom{s}{r} \right\}_{\substack{s \geq 1 \\ r \geq 0}} \cup \left\{ Z \binom{s_1, s_2}{r_1, r_2} \right\}_{\substack{s_1, s_2 \geq 1 \\ r_1, r_2 \geq 0}}$$

modulo the linear relations (1.2), (2.2) and those described in Remark 2.3 (iii).

(F1) We have

$$\begin{aligned} & \sum_{k \geq 0} \left(\dim_{\mathbb{Q}} \text{gr}_{k,1}^{\text{W,D}}(\mathcal{D}) y + \dim_{\mathbb{Q}} \text{gr}_{k,2}^{\text{W,D}}(\mathcal{D}) y^2 \right) x^k \\ & \equiv \chi_{\widetilde{M}}(x, y) \frac{1}{1 - \text{D}(x)y \text{O}_1(x) + \text{D}(x) \text{W}(x)y^2 - \text{A}(x)y^2} \pmod{y^3} \end{aligned}$$

where $\chi_{\widetilde{M}}(x, y) = 1 + \frac{x^2}{(1-x^2)^2} y + \frac{x^{12}}{(1-x^2)(1-x^4)(1-x^6)} y^2$, $\text{D}(x) = \frac{1}{(1-x^2)}$, $\text{O}_1(x) = \frac{x}{(1-x^2)}$ and

$$\begin{aligned} \text{W}(x) &= \sum_{k \geq 4} \left(\dim(M_k(\text{SL}_2(\mathbb{Z}))) + \dim(S_k(\text{SL}_2(\mathbb{Z}))) \right) x^k \\ \text{A}(x) &= \frac{x^8(1+x^6)}{(1-x^2)^2(1-x^6)^2}. \end{aligned}$$

(F2) The union of sets

$$\left\{ Z \binom{s}{r} \mid \begin{array}{l} s > r \geq 0 \\ s+r=k \end{array} \right\} \cup \left\{ Z \binom{s_1, s_2}{r_1, r_2} \mid \begin{array}{l} s_i > r_i \geq 0 \text{ for } i=1,2 \\ s_1+r_1 \text{ odd} \\ s_1+r_1+s_2+r_2=k \end{array} \right\} \quad (2.10)$$

gives a filtered basis for $\text{gr}_k^{\text{W}}(\mathcal{D})$ if k is odd. For even k the elements of depth 2 in (2.10) satisfy w_k linear relations, where w_k equals the coefficient of x^k in $\text{D}(x)\text{W}(x)$. Moreover, there are a_k symbols $Z_{\binom{s_1, s_2}{r_1, r_2}}$ with odd $s_1 + r_1$, where a_k equals the coefficient of x^k in $\text{A}(x)$, which complete (2.10) to a spanning set for $\text{gr}_k^{\text{W}}(\mathcal{D})$.

Remark 2.13. (i) We confirmed the conjecture for all weights up to 37.

(ii) We expect that $\chi_{\widetilde{M}}(x, y)$ is the bigraded Hilbert-Poincare series for the quasi-modular forms for $\text{SL}_2(\mathbb{Z})$.

(iii) The relations in (F2) that correspond to the Eisenstein series, are given by (2.5) and their derivations with respect to ∂ . For the moment it is not clear in which way the other relations coming from cusp forms are connected to the exotic relations described in Theorem 2.8.

(iv) For small weight representatives for those exceptional elements are $Z_{\binom{4,1}{1,2}}$, $Z_{\binom{5,1}{2,2}}$, $Z_{\binom{6,1}{1,2}}$, $Z_{\binom{6,1}{1,4}}$, $Z_{\binom{6,1}{3,2}}$ and $Z_{\binom{7,1}{2,2}}$.

(v) We like to mention that the series $\text{A}(x)$ counts the dimensions of the vector spaces spanned by primitive, alternal, swap-invariant polynomial bimoulds of degree $k - 2$.

(vi) Finally, for the combinatorial multiple Eisenstein series we expect by Conjecture 1.8 that (2.10) spans $\text{Fil}_{k,2}^{\text{W,D}}(\mathcal{Z}_q)$ and by the dimension conjecture in [6], we expect further relations, whose number equals the square of the dimension of cusp forms of weight k . Again, this has been confirmed with the computer for weights up to 70.

3 The interplay between q -zeta and zeta relations

We now study how the relations for double q -zeta values of the last section correlate to the relations satisfied by double zeta values. If not stated otherwise, the results in this section are obtained in [4].

Notation 3.1. Let A be a \mathbb{Q} -algebra. In the following $\mathcal{Z} = (\mathcal{Z}(X), \mathcal{Z}(X_1, X_2))$ denotes a mould of formal power series

$$\begin{aligned}\mathcal{Z}(X) &= \sum_{s \geq 1} Z(s) X^{s-1} \in A[[X]], \\ \mathcal{Z}(X_1, X_2) &= \sum_{s_1, s_2 \geq 1} Z(s_1, s_2) X_1^{s_1-1} X_2^{s_2-1} \in A[[X_1, X_2]].\end{aligned}$$

Definition 3.2. Let $\mathcal{Z} = (\mathcal{Z}(X), \mathcal{Z}(X_1, X_2))$ be a mould.

a) We say \mathcal{Z} satisfies the algebraic double shuffle relations, if

$$\begin{aligned}\mathcal{Z}(X_1) \mathcal{Z}(X_2) &= \mathcal{Z}(X_1, X_2) + \mathcal{Z}(X_2, X_1) + \frac{\mathcal{Z}(X_1) - \mathcal{Z}(X_2)}{X_1 - X_2} \\ &= \mathcal{Z}(X_1 + X_2, X_2) + \mathcal{Z}(X_1 + X_2, X_1) + Z(2).\end{aligned}$$

b) We say \mathcal{Z} satisfies the linear double shuffle relation, if

$$\mathcal{Z}(X_1, X_2) + \mathcal{Z}(X_2, X_1) + \frac{\mathcal{Z}(X_1) - \mathcal{Z}(X_2)}{X_1 - X_2} = \mathcal{Z}(X_1 + X_2, X_2) + \mathcal{Z}(X_1 + X_2, X_1) + \mathcal{Z}(2).$$

Of course, the generating series for (stuffle regularised) single and double zeta values satisfy the algebraic double shuffle relations, since $\zeta^*(1, k) = \zeta^{\sqcup}(1, k)$ for $k > 1$ and $0 = \zeta^{\sqcup}(1) = \zeta^*(1) = \zeta^{\sqcup}(1, 1) = \zeta^*(1, 1) + \zeta(2)/2$.

Proposition 3.3. If a mould $\mathcal{Z} = (\mathcal{Z}(X), \mathcal{Z}(X_1, X_2))$ satisfies the algebraic double shuffle relations, then the bimould $\tilde{\mathcal{Z}} = \left(\tilde{\mathcal{Z}}\binom{X}{Y}, \tilde{\mathcal{Z}}\binom{X_1, X_2}{Y_1, Y_2} \right)$ given by

$$\begin{aligned} \tilde{\mathcal{Z}}\binom{X}{Y} &:= \mathcal{Z}(X) + \mathcal{Z}(Y), \\ \tilde{\mathcal{Z}}\binom{X_1, X_2}{Y_1, Y_2} &:= \mathcal{Z}(X_1, X_2) + \mathcal{Z}(Y_1 + Y_2, Y_1) + \mathcal{Z}(X_2) \mathcal{Z}(Y_1) + \frac{1}{2} \mathcal{Z}\binom{2}{0} \end{aligned}$$

is symmetril and swap-invariant and thus satisfies the algebraic double q -shuffle relations.

Proof: The invariance under swap is checked easily. It remains to check symmetrility:

$$\begin{aligned} \tilde{\mathcal{Z}}\binom{X_1}{Y_1} \tilde{\mathcal{Z}}\binom{X_2}{Y_2} &= \mathcal{Z}(X_1) \mathcal{Z}(X_2) + \mathcal{Z}(Y_1) \mathcal{Z}(Y_2) + \mathcal{Z}(X_1) \mathcal{Z}(Y_2) + \mathcal{Z}(Y_1) \mathcal{Z}(X_2) \\ &= \mathcal{Z}(X_1, X_2) + \mathcal{Z}(X_2, X_1) + \frac{\mathcal{Z}(X_1) - \mathcal{Z}(X_2)}{X_1 - X_2} \\ &\quad + \mathcal{Z}(Y_1 + Y_2, Y_2) + \mathcal{Z}(Y_1 + Y_2, Y_1) + \mathcal{Z}\binom{2}{0} \\ &\quad + \mathcal{Z}(X_1) \mathcal{Z}(Y_2) + \mathcal{Z}(Y_1) \mathcal{Z}(X_2) \\ &= \tilde{\mathcal{Z}}\binom{X_1, X_2}{Y_1, Y_2} + \tilde{\mathcal{Z}}\binom{X_2, X_1}{Y_2, Y_1} + \frac{1}{X_1 - X_2} \left(\tilde{\mathcal{Z}}\binom{X_1}{Y_1 + Y_2} - \tilde{\mathcal{Z}}\binom{X_2}{Y_1 + Y_2} \right) \end{aligned}$$

□

Remark 3.4. (i) The bimould given by the lift of the generating series for (stuffle regularised) single and double zeta values satisfies Theorem 2.5 with $\partial \equiv 0$, therefore (2.7) implies Euler's formula for the even zeta values, once we know that $\zeta(2) = \frac{\pi^2}{6}$.

(ii) By [9], supplement to Proposition 5, there exists a solution $\beta = (\beta(X), \beta(X_1, X_2))$ to the algebraic double shuffle relations, where

$$\beta(X) = - \sum_{k \geq 2} \frac{B_k}{2k!} X^{k-1}$$

is a generating series for Bernoulli number. Then the symmetril and swap-invariant bimould $\tilde{\beta}$ needed for Theorem 1.13 is just its lift by means of Proposition 3.3.

Proposition 3.5. Assume the bimould $\mathcal{Z} = \left(\mathcal{Z}\binom{X}{Y}, \mathcal{Z}\binom{X_1, X_2}{Y_1, Y_2} \right)$ satisfies the algebraic double q -shuffle relations. If in addition $\mathcal{Z}\binom{k}{1} = 0$ for all $k > 1$, then the mould

$$\left(\mathcal{Z}\binom{X}{0}, \mathcal{Z}\binom{X_1, X_2}{0, 0} \right)$$

satisfies the algebraic double shuffle relations.

Proof: Obviously, we have

$$\begin{aligned}\mathcal{Z}\binom{X_1}{0}\mathcal{Z}\binom{X_2}{0} &= \mathcal{Z}\binom{X_1, X_2}{0,0} + \mathcal{Z}\binom{X_2, X_1}{0,0} + \frac{1}{X_1 - X_2} \left(\mathcal{Z}\binom{X_1}{0} - \mathcal{Z}\binom{X_2}{0} \right) \\ &= \mathcal{Z}\binom{X_1 + X_2, X_1}{0,0} + \mathcal{Z}\binom{X_1 + X_2, X_2}{0,0} + R\binom{X_1, X_2}{0,0},\end{aligned}$$

where

$$R\binom{X_1, X_2}{0,0} = \frac{\mathcal{Z}\binom{X_1 + X_2}{Y_1} - \mathcal{Z}\binom{X_1 + X_2}{Y_2}}{Y_1 - Y_2} \Big|_{Y_1 = Y_2 = 0} = \sum_{k \geq 1} Z\binom{k}{1} (X_1 + X_2)^{k-1}.$$

Since $Z\binom{1}{1} = Z\binom{2}{0}$, which holds by (2.3), the claim follows, since $Z\binom{k}{1} = 0$ for $k > 1$. \square

Proposition 3.6. If a bimould $\mathcal{Z} = \left(\mathcal{Z}\binom{X}{Y}, \mathcal{Z}\binom{X_1, X_2}{Y_1, Y_2} \right)$ satisfies the linear double q -shuffle relation, then the mould $\overline{\mathcal{Z}} = (\overline{\mathcal{Z}}(X), \overline{\mathcal{Z}}(X_1, X_2))$ given by the following power series

$$\begin{aligned}\overline{\mathcal{Z}}(X) &= \mathcal{Z}\binom{X}{0} - Z\binom{2}{0}X \\ \overline{\mathcal{Z}}(X_1, X_1) &= \mathcal{Z}\binom{X_1, X_2}{0,0} + \frac{1}{2}(X_1 - X_2) \frac{\mathcal{Z}'\binom{X_2}{0} - Z\binom{2}{0}}{X_2} + \frac{1}{2}X_1 \frac{\mathcal{Z}'\binom{X_1}{0} - Z\binom{2}{0}}{X_1},\end{aligned}$$

where

$$\mathcal{Z}'(X) = \sum_{k \geq 1} Z\binom{k}{1} X^{k-1}$$

satisfies the linear double shuffle relation.

Idea of proof: We can write $\mathcal{Z}'(X) = Z\binom{2}{0} + XF(X)$ for some power series F . Set

$$\epsilon(X_1, X_2) = \frac{1}{2}(X_1 - X_2)F(X_2) + \frac{1}{2}X_1F(X_1),$$

then a straightforward calculation gives

$$\epsilon(X_1 + X_2, X_2) + \epsilon(X_1 + X_2, X_1) - \epsilon(X_1, X_2) - \epsilon(X_2, X_1) = (X_1 + X_2)F(X_1 + X_2).$$

As before

$$\mathcal{Z}\binom{X_1 + X_2, X_1}{0,0} + \mathcal{Z}\binom{X_1 + X_2, X_2}{0,0} - \mathcal{Z}\binom{X_1, X_2}{0,0} - \mathcal{Z}\binom{X_2, X_1}{0,0} = R\binom{X_1, X_2}{0,0},$$

where using the above notation

$$\begin{aligned}R\binom{X_1, X_2}{0,0} &= \frac{\mathcal{Z}\binom{X_1}{0} - \mathcal{Z}\binom{X_2}{0}}{X_1 - X_2} - Z\binom{2}{0} - (X_1 + X_2)F(X_1 + X_2) \\ &= \frac{\overline{\mathcal{Z}}(X_1) + Z\binom{2}{0}X_1 - \overline{\mathcal{Z}}(X_1) - Z\binom{2}{0}X_2}{X_1 - X_2} - Z\binom{2}{0} - (X_1 + X_2)F(X_1 + X_2)\end{aligned}$$

Finally, collecting all those terms yields the claim, since

$$\overline{\mathcal{Z}}(X_1, X_2) = \mathcal{Z}\binom{X_1, X_2}{0,0} + \epsilon(X_1, X_2).$$

\square

Remark 3.7. If we apply this to the combinatorial multiple Eisenstein series $\mathcal{G} = (\mathcal{G}_1, \mathcal{G}_2)$, then its image $\overline{\mathcal{G}}$ equals the q -series realisation of the linear double shuffle relation due to Gangl-Kaneko-Zagier in [9], Theorem 7.

References

- [1] H. Bachmann: *Multiple Eisenstein series and q -analogues of multiple zeta values*, in *Periods in Quantum Field Theory and Arithmetic*, Springer Proceedings in Mathematics & Statistics 314, 237-258 (2020)
- [2] H. Bachmann: *The algebra of bi-brackets and regularized multiple Eisenstein series*, *J. Number Theory* 200, 260-294 (2019)
- [3] H. Bachmann, A. Burmester: *Combinatorial multiple Eisenstein series*, in preparation.
- [4] H. Bachmann, U. Kühn, N. Matthes: *TBA*, in preparation.
- [5] H. Bachmann, U. Kühn: *The algebra of multiple divisor functions and applications to multiple zeta values*, *Ramanujan J.* 40 (3), 605-648 (2016)
- [6] H. Bachmann, U. Kühn: *A dimension conjecture for q -analogues of multiple zeta values*, in *Periods in Quantum Field Theory and Arithmetic*, Springer Proceedings in Mathematics & Statistics 314, 237-258 (2020)
- [7] H. Bachmann, K. Tasaka: *The double shuffle relations for multiple Eisenstein series*, *Nagoya Math. J.* 230, 180-212, (2017)
- [8] J. I. Burgos Gil, J. Fresan, U. Kühn: *Classical multiple zeta values*, in *Multiple zeta values: from numbers to motives* edited by J. I. Burgos Gil, J. Fresan, to appear in "Clay Mathematics Proceedings".
- [9] H. Gangl, M. Kaneko, D. Zagier: *Double zeta values and modular forms*, *World Sci. Publ.* (2006), 71-106.
- [10] N. Matthes: *An algebraic characterization of the Kronecker function*, *Res. Math. Sci.* 6 (2019), no. 3, 6:24, 11.
- [11] L. Schneps: *ARI, GARI, Zig and Zag: An introduction to Ecalle's theory of multiple zeta values*, unpublished notes, arXiv:1507.01534 [math.NT]
- [12] K. Tasaka: *Hecke eigenform and double Eisenstein series*, *Proc. Amer. Math. Soc.*, 148(1) (2020), 53–58.
- [13] J. Zhao: *Uniform Approach to Double Shuffle and Duality Relations of Various q -Analogues of Multiple Zeta Values via Rota-Baxter Algebras*, in *Periods in Quantum Field Theory and Arithmetic*, Springer Proceedings in Mathematics & Statistics 314, 225-292 (2020)