# UNFOLDING THE DOUBLE SHUFFLE STRUCTURE OF q-MULTIPLE ZETA VALUES

## JAIME CASTILLO-MEDINA, KURUSCH EBRAHIMI-FARD and DOMINIQUE MANCHON $^{oxtimes}$

(Received 5 May 2014; accepted 20 November 2014)

#### **Abstract**

We exhibit the double *q*-shuffle structure for the *q*MZVs introduced by Ohno *et al.* ['Cyclic *q*-MZSV sum', *J. Number Theory* **132** (2012), 144–155].

2010 Mathematics subject classification: primary 11M32; secondary 11G55, 33D70.

*Keywords and phrases*: multiple zeta values, basic hypergeometric functions, *q*-analogue, shuffle relation, double shuffle.

#### 1. Introduction

In [17], Ohno *et al.* proposed for positive natural numbers  $n_1, n_2, ..., n_k \in \mathbb{N}$  and for any complex number q with |q| < 1 the following iterated infinite series:

$$\mathfrak{Z}_q(n_1,\ldots,n_k) := (1-q)^w \sum_{m_1 > \cdots > m_k > 0} \frac{q^{m_1}}{(1-q^{m_1})^{n_1} \cdots (1-q^{m_k})^{n_k}}$$
(1.1)

of depth  $k \ge 1$  and weight  $w := n_1 + \dots + n_k$  as a q-analogue of classical multiple zeta values (MZVs). Indeed, in the limit  $q \to 1$  the q-number  $[m]_q := (1 - q^m)(1 - q)^{-1}$  becomes  $m \in \mathbb{N}$  and the above infinite series reduces to the corresponding classical MZV of depth k and weight w, defined for positive natural numbers  $n_1, \dots, n_k \in \mathbb{N}$  by

$$\zeta(n_1, \dots, n_k) := \sum_{m_1 > \dots > m_k > 0} \frac{1}{m_1^{n_1} \cdots m_k^{n_k}}.$$
 (1.2)

The extra condition  $n_1 > 1$  is required in order that the right-hand side of (1.2) converges. The seminal works of Hoffman [12] and Zagier [26] initiated a systematic

The first author gratefully acknowledges support by the ICMAT Severo Ochoa Excellence Program and thanks ICMAT for warm hospitality during his visit. The second author is supported by a Ramón y Cajal research grant from the Spanish government. The second and third authors are supported by CNRS (GDR Renormalisation).

The second author is on leave from Université de Haute Alsace, Mulhouse, France,

<sup>© 2015</sup> Australian Mathematical Publishing Association Inc. 0004-9727/2015 \$16.00

study of MZVs. These real numbers appear in several contexts, for example arithmetic and algebraic geometry, algebra, combinatorics, mathematical physics, computer sciences, quantum groups and knot theory (see [5, 24, 25] for introductory reviews).

Kontsevich noticed that the series (1.2) has a simple representation in terms of iterated Riemann integrals [26]:

$$\zeta(n_1,\ldots,n_k) = \int_{0 < t_w < \cdots < t_1 < 1} \frac{dt_1}{\tau_1(t_1)} \cdots \frac{dt_w}{\tau_w(t_w)}, \tag{1.3}$$

where  $\tau_i(x) = 1 - x$  if  $i \in \{h_1, h_2, \dots, h_k\}$ ,  $h_j := n_1 + n_2 + \dots + n_j$ , and  $\tau_i(x) = x$  otherwise. Multiplying MZVs represented in either form, that is (1.2) or (1.3), results in  $\mathbb{Q}$ -linear combinations of MZVs. Hence, the  $\mathbb{Q}$ -vector space spanned by the real numbers (1.2) forms an algebra. The weight of a product of MZVs is defined as the sum of the weights. The product of MZVs arising from the sum representation (1.2) is usually called the stuffle, or quasi-shuffle, product. It preserves the weight, but is not homogeneous with respect to the depth. Euler's famous decomposition formula expresses the product of two single zeta values as

$$\zeta(a)\zeta(b) = \sum_{i=0}^{a-1} {i+b-1 \choose b-1} \zeta(b+i,a-i) + \sum_{j=0}^{b-1} {j+a-1 \choose a-1} \zeta(a+j,b-j).$$
 (1.4)

It is proven using integration by parts. As a result, from the interplay between the sum and the integral representations, products of MZVs can be written in two ways as  $\mathbb{Q}$ -linear combinations of MZVs. This leads to the so-called double shuffle relations among MZVs. The first example is given for a = 2 = b:

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

which implies  $\zeta(4) = 4\zeta(3, 1)$ . Let us also mention the regularisation, or Hoffman's, relations [15]. The simplest one is

$$\zeta(2,1) = \zeta(3) \tag{1.5}$$

and was already known to Euler. This is just the tip of an iceberg. The MZVs satisfy many relations over  $\mathbb Q$  and this gives rise to rich algebro-combinatorial structures. The latter are described abstractly in terms of so-called shuffle and quasi-shuffle (Hopf) algebras, which together encode the double shuffle relations for MZVs. We refer the reader to [14, 28] for detailed reviews of the algebraic structures related to MZVs.

In [6], we found a q-generalisation of Euler's decomposition formula [6, Corollary 12] for so-called modified q-multiple zeta values:

$$\bar{\mathfrak{z}}_q(n_1,\ldots,n_k) := (1-q)^{-w} \mathfrak{z}_q(n_1,\ldots,n_k) = \sum_{m_1 > \cdots > m_k > 0} \frac{q^{m_1}}{(1-q^{m_1})^{n_1} \cdots (1-q^{m_k})^{n_k}}$$
 (1.6)

of depth  $k \ge 1$  and weight  $w := n_1 + \cdots + n_k$  [17], expressing a product of two single modified q-zeta values of weights n and m in terms of double qMZVs. One can show

by multiplying both sides of this product by  $(1-q)^{n+m}$  that this formula reduces to Euler's formula (1.4) in the limit  $q \nearrow 1$ .

Several q-analogues of MZVs have appeared in the literature. The one proposed by Bradley [4], extending the definition of q-zeta function proposed by Kaneko et al. in [16] (see also [8]), has been studied in detail (see, for example, [17, 27, 28]) and can be related to linear combinations of series (1.1) (see [6]). Another q-analogue of MZVs, the algebra of multiple divisor functions, has been recently discovered by Bachmann and Kühn [2]. This version fits well with multiple Eisenstein series and modularity issues. In another model proposed by Schlesinger [22], the modified qMZVs  $\mathfrak{F}_q^S(n_1,\ldots,n_k)$  are defined by (1.1) with  $q^{m_1}$  replaced by 1 in the numerator. Finally, Okounkov [18] has proposed deep conjectures for yet another model in which the numerators are based on palindromic polynomials.

In this paper we shall complement the results in [6] by unfolding the double q-shuffle structure for the modified qMZVs defined in (1.6). In contrast to the classical q=1 case, these q-multiple zeta values  $\mathfrak{z}_q(n_1,\ldots,n_k)$  and  $\overline{\mathfrak{z}}_q(n_1,\ldots,n_k)$  make sense for any  $n_1,\ldots,n_k\in\mathbb{Z}$ , regardless of the sign. Hence, no further regularisation issues arise in this context. The q-quasi-shuffle structure is defined in terms of words with letters in an alphabet indexed by  $\mathbb{Z}$ , and the q-shuffle structure will be explained in terms of a particular weight -1 differential Rota-Baxter algebra [11] with invertible Rota-Baxter operator. We will use these double q-shuffle relations to derive an expression for  $\delta$ -terms in terms of modified qMZVs, where  $\delta$  stands for the derivation q(d/dq).

A double shuffle picture for q-multiple zeta values with positive arguments  $n_1, \ldots, n_k$  has also been indicated recently in the Bradley model by Takeyama [23]. Both approaches to the q-shuffle relations use a representation of q-multiple zeta values by a q-analogue of multiple polylogarithms with one variable. This representation is less direct in the Bradley model than in the Ohno-Okuda-Zudilin model, and needs a 'twisting' of the words (see [23, Lemma 2.10]), which is not needed in our approach.

The paper is organised as follows: after a quick review of the double shuffle structure for classical MZVs in Section 2, we introduce in Section 3 the Jackson integral J, the q-difference operator D defined by D[f](t) := f(t) - f(qt) and the q-summation operator P defined by  $P[f](t) := f(t) + f(qt) + f(q^2t) + \cdots$ . Operators P and D are mutually inverse in a suitable space of formal series. For any  $a, b \in \mathbb{Z}$ , explicit expressions for products  $P^a[f]P^b[g]$  are given in terms of  $P^i[P^j[f]g]$ ,  $P^i[fP^j[g]]$  and  $P^i[fg]$  for some  $i, j \in \mathbb{Z}$ .

In Section 4, we show how the modified Ohno–Okuda–Zudilin qMZVs can be expressed in terms of q-summation and q-difference operators, namely

$$\bar{\mathfrak{z}}_q(n_1,\ldots,n_k)=P^{n_1}[\bar{\mathfrak{y}}P^{n_2}[\bar{\mathfrak{y}}\cdots P^{n_k}[\bar{\mathfrak{y}}]\cdots]](q),$$

with  $\bar{y}(t) := t/(1-t)$ , and we give a complete picture of the double shuffle structure. The q-quasi-shuffle algebra is built on the space of words on the alphabet  $\widetilde{Y} := \{z_n, n \in \mathbb{Z}\}$ . The q-quasi-shuffle product H is the ordinary quasi-shuffle product, twisted in a certain sense by the operator  $T: z_j \mapsto z_j - z_{j-1}$ . The q-shuffle algebra consists of words with letters from the alphabet  $\widetilde{X} := \{d, y, p\}$ , all ending with y, and subject to

dp = pd = 1, so that one can also use the notation  $p^{-1} = d$ . The q-shuffle product is given recursively (with respect to the length of words) by

$$(yv) \coprod u = v \coprod (yu) = y(v \coprod u),$$

$$dv \coprod du = v \coprod du + dv \coprod u - d(v \coprod u),$$

$$pv \coprod pu = p(v \coprod pu) + p(pv \coprod u) - p(v \coprod u),$$

$$dv \coprod pu = pu \coprod dv = d(v \coprod pu) + dv \coprod u - v \coprod u$$

for any words v and u. We show that the product u is commutative and associative. It would be nice to have a purely combinatorial description of this product. In Section 5, the double shuffle relations are derived in the simple form

$$\begin{split} \overline{\mathfrak{z}}_{q}^{\text{\tiny III}}\left(\boldsymbol{v}\right) & \overline{\mathfrak{z}}_{q}^{\text{\tiny III}}\left(\boldsymbol{u}\right) = \overline{\mathfrak{z}}_{q}^{\text{\tiny III}}\left(\boldsymbol{v} \coprod \boldsymbol{u}\right), \\ \overline{\mathfrak{z}}_{q}^{\text{\tiny IH}}\left(\boldsymbol{v}'\right) & \overline{\mathfrak{z}}_{q}^{\text{\tiny IH}}\left(\boldsymbol{u}'\right) = \overline{\mathfrak{z}}_{q}^{\text{\tiny IH}}\left(\boldsymbol{v}' \coprod \boldsymbol{u}'\right) \end{split}$$

for any words v, u (respectively v', u') of letters from the alphabet  $\widetilde{X}$  (respectively  $\widetilde{Y}$ ), with

$$\overline{\mathfrak{z}}_q(n_1,\ldots,n_k)=\overline{\mathfrak{z}}_q^{\text{III}}(p^{n_1}y\cdots p^{n_k}y)=\overline{\mathfrak{z}}_q^{\text{IH}}(z_{n_1}\cdots z_{n_k}).$$

Finally, we give an explicit expression of  $\delta \bar{\mathfrak{z}}_q(n_1,\ldots,n_k)$  for any  $n_1,\ldots,n_k\in\mathbb{Z}$  and state a q-analogue of Hoffman's regularisation relations. Note that we have not explored possible Hopf algebra structures at this stage and that the limit for  $q\to 1$  still needs to be studied in detail. We plan to address these issues in a future work.

#### 2. Regularised double shuffle relations for MZVs

Let us briefly recall the double shuffle algebra for MZVs (for details, see [14, 24, 28]). In the introduction we have seen that MZVs are represented either by iterated sums (1.2) or in terms of iterated integrals (1.3). Thus, it is convenient to write them in terms of words. In view of (1.2) and (1.3), this can be done by using two alphabets:

$$X := \{x_0, x_1\}, \quad Y := \{y_1, y_2, y_3, \ldots\}.$$

We denote by  $X^*$ , respectively  $Y^*$ , the set of words with letters in X, respectively Y. The vector space  $\mathbb{Q}\langle X\rangle$ , which is freely generated by  $X^*$ , is a commutative algebra for the shuffle product. The vector space  $\mathbb{Q}\langle Y\rangle$ , freely generated by  $Y^*$ , is a commutative algebra for the quasi-shuffle product. In contrast to the shuffle product, the quasi-shuffle product involves extra terms coming from the semigroup structure of the alphabet Y and is not graded with respect to the length of words, but only filtered.

We denote by  $Y^*_{\text{conv}}$  the submonoid of words  $u = u_1 \cdots u_r$  with  $u_1 \neq y_1$  and we set  $X^*_{\text{conv}} := x_0 X^* x_1$ . An injective monoid morphism is given by changing the letter  $y_n$  into the word  $x_0^{n-1} x_1$ , namely

$$\mathfrak{s}: Y^* \longrightarrow X^*$$

$$y_{n_1} \cdots y_{n_r} \longmapsto x_0^{n_1 - 1} x_1 \cdots x_0^{n_r - 1} x_1.$$

It restricts to a monoid isomorphism from  $Y_{\text{conv}}^*$  onto  $X_{\text{conv}}^*$ . As the notation suggests,  $Y_{\text{conv}}^*$  and  $X_{\text{conv}}^*$  are two convenient ways to symbolise convergent MZVs through representations (1.2) and (1.3), respectively. Indeed, we can define

$$\zeta_{\text{IH}}\left(y_{n_1}\cdots y_{n_r}\right) := \zeta(n_1,\ldots,n_r) =: \zeta_{\text{III}}\left(\mathfrak{s}(y_{n_1}\cdots y_{n_r})\right)$$

and extend to finite linear combinations of convergent words by linearity. Clearly,  $\zeta_{\text{IM}} = \zeta_{\text{III}} \circ s$ . The map  $\zeta_{\text{IM}}$  defines an algebra homomorphism, giving the quasi-shuffle relations

$$\zeta_{\text{IH}} (u \coprod u') = \zeta_{\text{IH}} (u) \zeta_{\text{IH}} (u') \tag{2.1}$$

for any  $u, u' \in Y_{\text{conv}}^*$ . The map  $\zeta_{\text{III}}$  defines another algebra homomorphism, giving the shuffle relations

$$\zeta_{\text{III}}(v \coprod v') = \zeta_{\text{III}}(v)\zeta_{\text{III}}(v') \tag{2.2}$$

for any  $v, v' \in X^*_{\text{conv}}$ . By fixing an arbitrary value  $\theta$  to  $\zeta(1)$  and setting  $\zeta_{\text{IH}}(y_1) = \zeta_{\text{III}}(x_1) = \theta$ , it is possible to extend  $\zeta_{\text{IH}}$ , respectively  $\zeta_{\text{III}}$ , to all words in  $Y^*$ , respectively  $X^*x_1$ , such that (2.1), respectively (2.2), still hold. It is easy to show that for any words  $v \in X^*$  or  $u \in Y^*$ , the expressions  $\zeta_{\text{III}}(v)$  and  $\zeta_{\text{IH}}(u)$  are polynomials with respect to  $\theta$ . It is no longer true that the extended  $\zeta_{\text{IH}}$  coincides with the extended  $\zeta_{\text{III}} \circ \mathfrak{s}$ , but the defect can be described explicitly.

**THEOREM** 2.1 (L. Boutet de Monvel [26]). There exists an infinite-order invertible differential operator  $\rho : \mathbb{R}[\theta] \to \mathbb{R}[\theta]$  such that

$$\zeta_{\text{III}} \circ \mathfrak{s} = \rho \circ \zeta_{\text{ITI}}$$
.

The operator  $\rho$  is explicitly given by the series

$$\rho = \exp\left(\sum_{n>2} \frac{(-1)^n \zeta(n)}{n} \left(\frac{d}{d\theta}\right)^n\right).$$

In particular,  $\rho(1) = 1$ ,  $\rho(\theta) = \theta$  and, more generally,  $\rho(L) - L$  is a polynomial of degree smaller than d - 2 if L is of degree d; hence,  $\rho$  is invertible. A proof of Theorem 2.1 can be found, for example, in [5, 15, 19].

Any word  $u \in Y_{\text{conv}}^*$  gives rise to Hoffman's regularisation relation

$$\zeta_{\text{III}}(x_1 \coprod \mathfrak{s}(u) - \mathfrak{s}(y_1 \coprod u)) = 0, \tag{2.3}$$

which is a direct consequence of Theorem 2.1. This linear combination of words is convergent; hence, (2.3) is a relation between convergent MZVs, although divergent ones have been used to establish it. The simplest regularisation relation,  $\zeta(2, 1) = \zeta(3)$ , is obtained by applying (2.3) to the word  $u = y_2$ .

#### 3. The Jackson integral

The results in [6] are essentially based on replacing the classical indefinite Riemann integral  $R[f](t) := \int_0^t f(y) dy$  in (1.3) by its q-analogue, known as Jackson's integral:

$$J[f](t) := (1 - q) \sum_{n > 0} f(q^n t) q^n t.$$
(3.1)

Rota [20, 21] gave an elementary algebraic description of the map J in terms of the q-dilation operator E[f](t) := f(qt), together with the multiplication operator  $M_f[g](t) := (fg)(t) = f(t)g(t)$ , such that

$$J[f](t) = (1 - q) \sum_{n>0} E_q^n [M_{id}[f]](t) =: (1 - q)PM_{id}[f](t).$$
 (3.2)

One can recover the ordinary Riemann integral as the limit of the Jackson integral for  $q \nearrow 1$ . Note however that the Jackson integral makes sense purely algebraically if q is considered as an indeterminate: more precisely, let  $\mathcal{A} = t\mathbb{Q}[[t,q]]$  be the space of formal series in two variables with strictly positive valuation in t. We can see  $\mathcal{A}$  as the space of series in t without constant term and with coefficients in  $\mathbb{Q}[[q]]$ . Then (3.1) defines the Jackson integral as a  $\mathbb{Q}[[q]]$ -linear endomorphism of  $\mathcal{A}$ . The  $\mathbb{Q}[[q]]$ -linear map  $P: \mathcal{A} \to \mathcal{A}$ , defined by

$$P[f](t) := \sum_{n>0} E^n[f] = f(t) + f(qt) + f(q^2t) + f(q^3t) + \cdots,$$

satisfies the Rota-Baxter identity of weight -1:

$$P[f]P[g] = P[P[f]g] + P[fP[g]] - P[fg]. \tag{3.3}$$

We refer the reader to [6] and [10, 20, 21] for more details regarding Rota–Baxter algebras and related topics (note that the map P is denoted by  $\tilde{P}_q$  in [6]). From this, it follows that Jackson's integral (3.2) satisfies the relation

$$J[f]J[g] = J[J[f]g + f J[g] - (1 - q) idfg].$$

Or, equivalently,

$$J[f]J[g] = J[fJ[g]] + aJ[J[E[f]]g],$$

which is commonly considered to be the q-analogue for the classical integration by parts rule:

$$R(f)R(g) = R(fR(g) + R(f)g),$$

which can be seen as dual to Leibniz' rule for derivations. The inverse of the map P is defined in terms of the finite q-difference operator:

$$D := I - E$$

where I is the identity map, I[f] := f. It is easy to see that D satisfies the generalised Leibniz rule for finite differences:

$$D[fg] = D[f]g + fD[g] - D[f]D[g]. (3.4)$$

This makes  $\mathcal{A}$  a weight -1 differential Rota-Baxter algebra [11], with the crucial additional property that P and D are mutually inverse. Interestingly, (3.4) can be reordered:

$$D[f]D[g] = D[f]g + fD[g] - D[fg], (3.5)$$

thus showing a striking similarity with (3.3). This will play a crucial role in the remainder of this paper. For positive  $a, b \in \mathbb{N}$ , the generalised Leibniz rule (3.5) leads to the recursion

$$D^{a}[f]D^{b}[g] = D^{a-1}[f]D^{b}[g] + D^{a}[f]D^{b-1}[g] - D[D^{a-1}[f]D^{b-1}[g]].$$

From this, we deduce the following theorem.

Theorem 3.1. Let  $1 < a \le b \in \mathbb{N}$ . Then

$$D^{a}[f]D^{b}[g] = \sum_{j=0}^{a-1} \sum_{i=1}^{b-j} (-1)^{j} \binom{a+b-1-i-j}{j, a-1-j, b-i-j} D^{j}[fD_{q}^{i}[g]]$$

$$+ \sum_{j=1}^{a} \sum_{i=1}^{b-j} (-1)^{j} \binom{a+b-1-i-j}{j-1, a-j, b-i-j} D^{j}[fD_{q}^{i}[g]]$$

$$+ \sum_{j=0}^{b-1} \sum_{i=1}^{a-j} (-1)^{j} \binom{a+b-1-i-j}{j, b-1-j, a-i-j} D^{j}[D_{q}^{i}[f]g]$$

$$+ \sum_{j=1}^{b} \sum_{i=1}^{a-j} (-1)^{j} \binom{a+b-1-i-j}{j-1, b-j, a-i-j} D^{j}[D_{q}^{i}[f]g]$$

$$+ \sum_{i=1}^{a} (-1)^{j} \binom{a+b-1-j}{j-1, a-j, b-j} D^{j}[fg]. \tag{3.6}$$

**PROOF.** The proof of (3.6) follows the same lines as in [9]; see also [6]. We briefly recall the basic idea [9]. Identity (3.5) can be represented pictorially:

$$\downarrow$$
 =  $\downarrow$  +  $\downarrow$  -  $\downarrow$  ,

where the bullets represent the operator D. The branching indicates multiplication—we skipped the decoration of the left and right leaves by f and g, respectively. Observe that each of the trees on the right-hand side has one dot less than the tree on the left-hand side.

We define  $\Gamma(a,b,c;f,g) := D_q^c(D_q^a(f)D_q^b(g))$ , which would be represented by a tree with a dots on the left-hand branch, b dots on the right-hand branch and c dots on the upper branch. Using (3.5), we try to eliminate the dots on the lower branches, that is, to write  $\Gamma(a,b,c;f,g)$  as a sum of the three terms  $\Gamma(0,i,c+j;f,g)$ ,  $\Gamma(i,0,c+j;f,g)$  and  $\Gamma(0,0,c+j;f,g)$ .

<sup>&</sup>lt;sup>1</sup>In a differential Rota–Baxter algebra with differential D and Rota–Baxter operator P, the equality  $D \circ P = \text{Id holds but } P \circ D = \text{Id does not hold in general.}$ 

Hence, starting with a dots on the left-hand branch, b dots on the right-hand branch and c dots on the upper branch, Díaz and Páez [9] described the counting of possibilities of reducing the number of dots on either of the lower branches in terms of 'moving' dots successively upwards. Identity (3.5) implies essentially three moves, two of which eliminate a dot on either of the lower branches. The last move merges a dot from each branch into a new dot, which is then lifted upwards. The coefficients in (3.6) result from carefully counting the moves needed to get to either of the three terms  $\Gamma(0, i, c + j; f, g)$ ,  $\Gamma(i, 0, c + j; f, g)$  and  $\Gamma(0, 0, c + j; f, g)$ .

Note that the above expression can be simplified to the following more convenient relation.

Proposition 3.2. Let  $1 < a \le b \in \mathbb{N}$ . Then

$$D^{a}[f]D^{b}[g] = \sum_{j=0}^{a} \sum_{i=1}^{b-j} (-1)^{j} \binom{a+b-1-i-j}{a-1} \binom{a}{j} D^{j}[fD_{q}^{i}[g]]$$

$$+ \sum_{j=0}^{b} \sum_{i=1}^{\max(1,a-j)} (-1)^{j} \binom{a+b-1-i-j}{b-1} \binom{b}{j} D^{j}[D_{q}^{i}[f]g]$$

$$+ \sum_{j=1}^{a} (-1)^{j} \binom{a+b-1-j}{j-1,a-j,b-j} D^{j}[fg].$$

**PROOF.** The proof of this follows the same arguments as in [6]. By exchanging the order of summation in each of the terms in (3.6), we can combine the first and second terms and the third and fourth terms. Then some basic binomial identities are used.  $\Box$ 

A natural question to ask is, whether we can resolve products, like D[f]P[g]. From (3.4), we conclude quickly that

$$D[f]P[g] = D[fP[g]] + D[f]g - fg. (3.7)$$

Equations (3.3), (3.4) and (3.7) are equivalent. The recursion for a general product of this form is given by

$$D^a[f]P^b[g] = D[D^{a-1}[f]P^b[g]] + D^a[f]P^{b-1}[g] - D^{a-1}[f]P^{b-1}[g],$$

which leads to a closed expression.

Proposition 3.3. Let  $1 < a \le b \in \mathbb{N}$ . Then

$$D^{a}[f]P^{b}[g] = \sum_{j=0}^{a} \sum_{i=1}^{b-a+j} (-1)^{a-j} \binom{b-1-i+j}{a-1} \binom{a}{j} D^{j}[fP_{q}^{i}[g]]$$

$$+ \sum_{k=1}^{a} \sum_{i=1}^{k} (-1)^{a-k} \binom{b-1-i+k}{b-1} \binom{b}{a-k} D^{k-i}[D_{q}^{i}[f]g]$$

$$+ \sum_{j=0}^{a-1} (-1)^{a-j} \binom{b-1+j}{j} D^{j}[fg]. \tag{3.8}$$

PROOF. Again this follows the same argument given in the proof of (3.6). See [6, 9].

We will see below that these identities provide q-generalisations of Euler's decomposition formula for the modified q-analogue (1.6) at values  $n_1, n_2, \ldots, n_k \in \mathbb{Z}$ .

### 4. *q*-Analogues of multiple zeta values

Following [6], we define the functions x, y and  $\bar{y}$  by

$$x(t) = \frac{1}{t}, \quad y(t) = \frac{1}{1-t}, \quad \bar{y}(t) = \frac{t}{1-t}.$$

Recall the common notation for *q*-numbers,  $[m]_q := (1 - q^m)/(1 - q)$ .

**4.1. Iterated Jackson integrals and** *q***-multiple zeta values.** Replacing the Riemann integrals in (1.3) by Jackson integrals (3.2), we arrive at a *q*-analogue of MZVs, which was considered by Ohno *et al.* in [17]. It is defined for positive natural numbers  $n_i \in \mathbb{N}$ ,  $n_1 > 1$ ,  $w := n_1 + \cdots + n_k$ , in terms of iterated Jackson integrals evaluated at *q*:

$$\mathfrak{Z}_q(n_1,\ldots,n_k):=J[\rho_1J[\rho_2\cdots J[\rho_w]\cdots]](q),$$

where  $\rho_i(t) = y(t)$  if  $i \in \{h_1, h_2, \dots, h_k\}$ ,  $h_j := n_1 + n_2 + \dots + n_j$ , and  $\rho_i(t) = x(t)$  otherwise. Writing this out in detail yields

$$\mathfrak{z}_{q}(n_{1},\ldots,n_{k}) = (1-q)^{w} \underbrace{P\left[P\left[\cdots P\left[\bar{y}\cdots P\left[P\left[\cdots P\left[\bar{y}\right]\right]\right]\right]\right]\cdots\right]\right]}_{n_{1}}(q)$$

$$= \sum_{m_{1}>\cdots>m_{k}>0} \frac{q^{m_{1}}}{\left[m_{1}\right]_{q}^{n_{1}}\cdots\left[m_{k}\right]_{q}^{n_{k}}}.$$

$$(4.1)$$

In the introduction, we mentioned the modified qMZV:

$$(1-q)^{w}\bar{\mathfrak{z}}_{q}(n_{1},\ldots,n_{k})=\mathfrak{z}_{q}(n_{1},\ldots,n_{k}). \tag{4.2}$$

In the following, we will mainly work with these modified qMZVs. From (4.1), it is clear that

$$\bar{\mathfrak{z}}_q(n_1,\ldots,n_k)=P^{n_1}[\bar{\mathfrak{y}}\cdots P^{n_k}[\bar{\mathfrak{y}}]\cdots](q).$$

**4.2.** Convergence issues and extension to integer arguments of any sign. Observe that

$$\bar{\mathfrak{z}}_q(0) = P^0[\bar{y}](q) = \sum_{m>0} q^m = \bar{y}(q) = \frac{q}{1-q},$$

which makes sense as a formal series in q, the specialisation of which is well defined for any complex q with |q| < 1. More generally, (4.1) and (4.2) make sense as an element of  $q\mathbb{Q}[[q]]$ , that is, as a formal series in q without constant term, for any

 $n_1, \ldots, n_k \in \mathbb{Z}$ , and the series converges for a complex number q with |q| < 1. This follows from

$$\begin{aligned} |\bar{\mathfrak{z}}_{q}(n_{1},\ldots,n_{k})| &\leq \sum_{m_{1}>\cdots>m_{k}>0} \frac{|q|^{m_{1}}}{(1-|q|^{m_{1}})^{n_{1}}\cdots(1-|q|^{m_{k}})^{n_{k}}} \\ &\leq \sum_{m_{1}>\cdots>m_{k}>0} \frac{|q|^{m_{1}}}{(1-|q|)^{|n_{1}|}\cdots(1-|q|)^{|n_{k}|}} \\ &\leq (1-|q|)^{-\tilde{w}} \sum_{m'_{1},\ldots,m'_{k}>0} |q|^{m'_{1}+\cdots+m'_{k}} \end{aligned}$$

with  $\tilde{w} = \sum_{i=1}^k |n_i|$  and hence  $|\bar{\mathfrak{z}}_q(n_1,\ldots,n_k)| \le |q|^k (1-|q|)^{-\tilde{w}-k}$ . Also, for nonmodified qMZVs,

$$|\mathfrak{z}_q(n_1,\ldots,n_k)| \le |q|^k (1-|q|)^{-\tilde{w}-k} |1-q|^w.$$

PROPOSITION 4.1. For  $n_1 \ge 2$  and  $n_2, \ldots, n_k \ge 1$ , as  $q \to 1$  with |q| < 1 and  $Arg(1 - q) \in [-\pi/2 + \varepsilon, \pi/2 - \varepsilon]$  for some  $\varepsilon > 0$ , the k-fold iterated sum (4.1) converges to the corresponding classical MZV of depth k and weight w.

PROOF. This is an immediate application of Abel's limit theorem for power series with radius of convergence 1 [1, pages 41–42].

The q-parameter may then be considered a regularisation of MZVs for arguments in  $\mathbb{Z}$ . From the definition,

$$\bar{\mathfrak{z}}_q(0,0) = \sum_{m_1 > m_2 > 0} q^{m_1} = \sum_{m > 0} (m-1)q^m = \left(\frac{q}{1-q}\right)^2, \qquad \bar{\mathfrak{z}}_q(0,\ldots,0) = \left(\frac{q}{1-q}\right)^k.$$

Using  $D = P^{-1}$ , we see that for a < 0,

$$\bar{\mathfrak{z}}_q(a) = D^{|a|}(\bar{\mathfrak{y}})(q) = \sum_{m>0} q^m (1 - q^m)^{|a|}$$

and, for a > 0,

$$\bar{\mathfrak{z}}_q(a,0) = \sum_{m_1 > m_2 > 0} \frac{q^{m_1}}{(1 - q^{m_1})^a} = \sum_{m > 0} \frac{(m-1)q^m}{(1 - q^m)^a}.$$

Finally, it will be convenient to express our qMZVs in terms of  $q^{-1}$  whenever possible.

PROPOSITION 4.2. The q-multiple zeta values  $\mathfrak{z}_q(n_1,\ldots,n_k)$  and  $\overline{\mathfrak{z}}_q(n_1,\ldots,n_k)$  make sense as a series in  $\mathbb{Q}[[q^{-1}]]$  for any  $(n_1,\ldots,n_k)$  with  $n_j \geq 1$  and  $n_1 \geq 2$ .

**Proof.** This comes from a straightforward computation:

$$\mathfrak{Z}_q(n_1,\ldots,n_k) = \sum_{m_1 > \cdots > m_k > 0} \frac{(q^{-1})^{-m_1}(q^{-1})^{(m_1-1)n_1 + \cdots + (m_k-1)n_k}}{[m_1]_{q^{-1}}^{n_1} \cdots [m_k]_{q^{-1}}^{n_k}}.$$

**4.3.** The *q*-shuffle structure. Let *W* be the set of words on the alphabet  $\widetilde{X} := \{d, y, p\}$  ending with *y*, subject to dp = pd = 1 (where 1 stands for the empty word). We shall also use the notation  $p^{-1} = d$ . Any nonempty word *v* in *W* can be written uniquely as

$$v = p^{n_1} y \cdots p^{n_k} y$$

with k > 0 and  $n_1, \ldots, n_k \in \mathbb{Z}$ . The length of the word v is given by  $\ell(v) = k + |n_1| + \cdots + |n_k|$ . For later use, we introduce the notation

$$\bar{\mathfrak{z}}_{q}^{\text{III}}(p^{n_{1}}y\cdots p^{n_{k}}y) := \bar{\mathfrak{z}}_{q}(n_{1},\ldots,n_{k}), 
\mathfrak{z}_{q}^{\text{III}}(p^{n_{1}}y\cdots p^{n_{k}}y) := \mathfrak{z}_{q}(n_{1},\ldots,n_{k}).$$

The *q*-shuffle product is given on  $\mathbb{Q}$ . W recursively (with respect to the length of words) by  $\mathbf{1} \coprod v = v \coprod \mathbf{1} = v$  for any word v and

$$(yv) \coprod u = v \coprod (yu) = y(v \coprod u), \tag{4.3}$$

$$pv \coprod pu = p(v \coprod pu) + p(pv \coprod u) - p(v \coprod u), \tag{4.4}$$

$$dv \coprod du = v \coprod du + dv \coprod u - d(v \coprod u), \tag{4.5}$$

$$dv \coprod pu = pu \coprod dv = d(v \coprod pu) + dv \coprod u - v \coprod u$$
 (4.6)

for any words v and u in W. Equations (4.4), (4.5) and (4.6) come from an abstraction of (3.3), (3.4) and (3.7), respectively.

**THEOREM** 4.3. The q-shuffle product is commutative and associative. Moreover, for any  $v, u \in W$ ,

$$\bar{\mathfrak{Z}}_q^{\coprod}(v)\bar{\mathfrak{Z}}_q^{\coprod}(u)=\bar{\mathfrak{Z}}_q^{\coprod}(v\coprod u).$$

**PROOF.** Commutativity follows easily from  $u \coprod v = v \coprod u$  and induction on the sum  $\ell(u) + \ell(v)$  of the lengths of the two words u and v. We sketch the proof of the associativity relation  $(u \coprod v) \coprod z = u \coprod (v \coprod z)$  by induction on the sum  $\ell(u) + \ell(v) + \ell(z)$  of the lengths of the three words u, v and v.

If one of the words is empty, there is nothing to prove. Otherwise we write  $u = \alpha a$ ,  $v = \beta b$  and  $z = \gamma c$ , where  $\alpha$ ,  $\beta$  or  $\gamma$  can be the letters p, d or y. This yields theoretically 27 different cases, which however will reduce substantially.

• First case: one of the letters is a y. Using (4.3) repeatedly as well as the induction hypothesis,

$$(ya \coprod v) \coprod z = (y(a \coprod v)) \coprod z = y((a \coprod v) \coprod z) = y(a \coprod (v \coprod z)) = ya \coprod (v \coprod z).$$

There are a number of similar cases which reduce to this one by using commutativity.

• Second case:  $\alpha = \beta = \gamma = d$ . We use (4.5) repeatedly as well as commutativity, and we freely omit parentheses when using the induction hypothesis. On one

hand.

$$(da \coprod db) \coprod dc = (a \coprod db + da \coprod b - d(a \coprod b)) \coprod dc$$

$$= a \coprod db \coprod dc + b \coprod da \coprod dc - d(a \coprod b) \coprod dc$$

$$= a \coprod (b \coprod dc + db \coprod c - d(b \coprod c)) + b \coprod (a \coprod dc + da \coprod c)$$

$$- d(a \coprod c)) - a \coprod b \coprod dc - d(a \coprod b) \coprod c + d(a \coprod b \coprod c)$$

$$= \underbrace{a \coprod db \coprod c - a \coprod d(b \coprod c)}_{1} + \underbrace{b \coprod a \coprod dc}_{3} + \underbrace{b \coprod da \coprod c}_{4}$$

$$- \underbrace{b \coprod d(a \coprod c)}_{5} - \underbrace{d(a \coprod b) \coprod c}_{6} + \underbrace{d(a \coprod b \coprod c)}_{7} .$$

On the other hand,

$$da \coprod (db \coprod dc) = da \coprod (b \coprod dc + db \coprod c - d(b \coprod c))$$

$$= da \coprod dc \coprod b + da \coprod db \coprod c - da \coprod d(b \coprod c)$$

$$= a \coprod dc \coprod b + da \coprod c \coprod b - d(a \coprod c) \coprod b + a \coprod db \coprod c$$

$$+ da \coprod b \coprod c - d(a \coprod b) \coprod c - a \coprod d(b \coprod c)$$

$$- da \coprod b \coprod c + d(a \coprod b \coprod c).$$

$$= \underbrace{a \coprod dc \coprod b}_{3} - \underbrace{d(a \coprod c) \coprod b}_{5} + \underbrace{a \coprod db \coprod c}_{4} + \underbrace{da \coprod b \coprod c}_{4}$$

$$- \underbrace{d(a \coprod b) \coprod c}_{6} - \underbrace{a \coprod d(b \coprod c)}_{2} + \underbrace{d(a \coprod b \coprod c)}_{5}.$$

Hence, the two expressions coincide.

There are three more cases to consider and they are treated by similar computations (see [7]).

- Third case: one letter p and two letters d.
- Fourth case: two letters p and one letter d.
- Fifth case:  $\alpha = \beta = \gamma = p$ .

Now let us call a differential Rota–Baxter algebra *invertible* if the Rota–Baxter operator P and the differential D are mutually inverse. Then ( $\mathbb{Q}.W, \mathbb{H}$ ) is the free invertible differential Rota–Baxter algebra of weight -1 with one generator. Indeed, the generator is y, the Rota–Baxter operator (respectively the differential) is left concatenation by the letter p (respectively d) and identities (4.3)–(4.6) guarantee the weight -1 differential Rota–Baxter identities. This object is rather different from (and much smaller than) the free differential Rota–Baxter algebra with one generator constructed in [11]. The map

$$\mathcal{Z}: \mathbb{Q} \cdot W \longrightarrow \mathcal{A}$$

$$p^{n_1} y \cdots p^{n_k} y \longmapsto P^{n_1} [\bar{y} P^{n_2} [\bar{y} \cdots P^{n_k} [\bar{y}] \cdots]]$$

is the unique map of invertible differential Rota–Baxter algebras of weight -1 such that  $Z(y) = \bar{y}$  (recall that  $\bar{y}(t, q) = \bar{y}(t) := t/(1 - t)$ ). The second assertion of Theorem 4.3 immediately comes from the fact that for any word v,

$$\bar{\mathfrak{Z}}_{q}^{\mathrm{III}}(v) = \mathcal{Z}(v)(t,q)|_{t=q}.$$

REMARK 4.4. Considering what happens with ordinary shuffle or quasi-shuffle products, it would be nice to have a purely combinatorial interpretation of the product III. Theorem 4.3 would obviously have an immediate proof if the map  $\mathbb{Z}$  were injective, but we have not been able to prove this.

**4.4. Euler decomposition formulas.** Recall the identities (3.7) and (3.8) in Propositions 3.2 and 3.3, respectively, from which we derive a q-generalisation of Euler's decomposition formulas for qMZVs to complement [6, Corollary 12]. For  $1 < a \le b$ ,

$$\bar{\mathfrak{z}}_{q}(-a)\bar{\mathfrak{z}}_{q}(-b) = \sum_{j=0}^{a} \sum_{i=1}^{b-j} (-1)^{j} \binom{a+b-1-i-j}{a-1} \binom{a}{j} \bar{\mathfrak{z}}_{q}(-j,-i) 
+ \sum_{j=0}^{b} \sum_{i=1}^{\max(1,a-j)} (-1)^{j} \binom{a+b-1-i-j}{b-1} \binom{b}{j} \bar{\mathfrak{z}}_{q}(-j,-i) 
+ \sum_{j=1}^{a} (-1)^{j} \binom{a+b-1-j}{j-1,a-j,b-j} \bar{\mathfrak{z}}_{q}(-j,0)$$

and

$$\bar{\mathfrak{z}}_{q}(-a)\bar{\mathfrak{z}}_{q}(b) = \sum_{j=0}^{a} \sum_{i=1}^{b-a+j} (-1)^{a-j} \binom{b-1-i+j}{a-1} \binom{a}{j} \bar{\mathfrak{z}}_{q}(-j,i) 
+ \sum_{k=1}^{a} \sum_{i=1}^{k} (-1)^{a-k} \binom{b-1-i+k}{b-1} \binom{b}{a-k} \bar{\mathfrak{z}}_{q}(-k+1,-i) 
+ \sum_{j=0}^{\min(a-1,b-a+1)} (-1)^{a-j} \binom{b-1+j}{j,a-1-j,b-a-j} \bar{\mathfrak{z}}_{q}(-j,0).$$

In [6], we have explained how the  $\delta := q(d/dq)$  derivation terms appear in the q-generalisation of Euler's decomposition formula. Below, in subsection 4.6, we will show how for j > 0 one can rewrite the third summands on the right-hand side of each of the above identities in terms of linear combinations of modified qMZVs and derivation terms  $\delta_{3q}$ .

**4.5.** The *q*-quasi-shuffle structure. In [6], we used the sum representation (4.1) of the product of two modified qMZVs of weight a, b > 1 to obtain the following identity:

$$\bar{\mathfrak{z}}_{q}(a)\bar{\mathfrak{z}}_{q}(b) = \bar{\mathfrak{z}}_{q}(a,b) + \bar{\mathfrak{z}}_{q}(b,a) + \bar{\mathfrak{z}}_{q}(a+b) - \bar{\mathfrak{z}}_{q}(a,b-1) - \bar{\mathfrak{z}}_{q}(b,a-1) - \bar{\mathfrak{z}}_{q}(a+b-1).$$

It is easily seen that the same computation holds for any  $a, b \in \mathbb{Z}$ . We can formulate the above q-quasi-shuffles in terms of a quasi-shuffle-like algebra.

Let  $\widetilde{Y}$  be the alphabet  $\{z_n, n \in \mathbb{Z}\}$ . We denote by  $\widetilde{Y}^*$  the set of words with letters in  $\widetilde{Y}$ , and by  $\mathbb{Q}\langle \widetilde{Y} \rangle$  the free associative algebra on  $\widetilde{Y}$ , which is freely generated as a  $\mathbb{Q}$ -vector space by  $\widetilde{Y}^*$ . We equip  $\widetilde{Y}$  with the internal commutative associative product  $[z_i z_j] := z_{i+j}$ . For later use, we introduce the notation

$$\bar{\mathfrak{z}}_{q}^{\text{IH}}(z_{n_{1}}\cdots z_{n_{k}}) := \bar{\mathfrak{z}}_{q}(n_{1},\ldots,n_{k}),$$
 $\mathfrak{z}_{q}^{\text{IH}}(z_{n_{1}}\cdots z_{n_{k}}) := \mathfrak{z}_{q}(n_{1},\ldots,n_{k}).$ 

On  $\mathbb{Q}\langle \tilde{Y} \rangle$ , we consider the ordinary quasi-shuffle product \*, recursively defined by

$$av * bv' := a(v * bv') + b(av * v') + [ab](v * v').$$

This product is known to be commutative and associative [13]. Now we consider the linear operator T on  $\mathbb{Q}\langle \tilde{Y} \rangle$  defined by

$$T(z_n v) := z_n v - z_{n-1} v.$$

It is obviously injective. For any  $m, n \in \mathbb{Z}$  and for any  $u, v \in \widetilde{Y}^*$ , we compute

$$T(z_m u) * T(z_n v) = (z_m - z_{m-1})u * (z_n - z_{n-1})v$$

$$= (z_m - z_{m-1})(u * (z_n - z_{n-1})v) + (z_n - z_{n-1})(v * (z_m - z_{m-1})u)$$

$$+ ((z_{m+n} - z_{m+n-1}) - (z_{m+n-1} - z_{m+n-2}))(u * v)$$

$$= T(z_m (u * T(z_n v)) + z_n (T(z_m u) * v)) + T(z_{m+n} (u * v)).$$

We then define our q-quasi-shuffle product by  $T(u \coprod v) = Tu * Tv$  for any words u, v. In view of the computation above,

$$z_m u \coprod z_n v = z_m (u * T(z_n v)) + z_n (T(z_m u) * v) + (z_{m+n} - z_{m+n-1})(u * v).$$

In particular,

$$z_m \coprod z_n = z_m(Tz_n) + z_n(Tz_m) + Tz_{m+n}$$
  
=  $z_m z_n + z_n z_m + z_{m+n} - z_m z_{n-1} - z_n z_{m-1} - z_{m+n-1}$ .

Proposition 4.5. The q-quasi-shuffle product  $\coprod$  is commutative and associative. Moreover, for any  $u, v \in Y$ ,

$$\bar{\mathfrak{z}}_q^{\scriptscriptstyle{\mathsf{IH}}}\left(u\right)\bar{\mathfrak{z}}_q^{\scriptscriptstyle{\mathsf{IH}}}\left(v\right)=\bar{\mathfrak{z}}_q^{\scriptscriptstyle{\mathsf{IH}}}\left(u\bowtie v\right).$$

**PROOF.** Commutativity and associativity of  $\mathbb{H}$  come from the injectivity of T and from the fact that the ordinary quasi-shuffle product \* is commutative and associative. The second assertion has been already shown when u and v are two letters. The

computation for two words is entirely similar:

$$\begin{split} & \frac{3_{q}^{\text{IH}}}{l} \left( z_{n_{1}} \cdots z_{n_{r}} \right) \overline{\delta}_{q}^{\text{IH}} \left( z_{n_{r+1}} \cdots z_{n_{r+s}} \right) \\ & = \sum_{\substack{k_{1} > \cdots > k_{r} \\ k_{r+1} > \cdots > k_{r+s}}} \frac{q^{k_{1} + k_{r+1}}}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}} \\ & = \sum_{\substack{k_{1} > k_{r+1}, k_{1} > \cdots > k_{r} \\ k_{r+1} > \cdots > k_{r+s}}} \frac{q^{k_{1} + k_{r+1}}}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}} \\ & + \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r} \\ k_{r+1} > \cdots > k_{r+s}}} \frac{q^{k_{1} + k_{r+1}}}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}} \\ & + \sum_{\substack{k_{1} = k_{r+1}, k_{1} > \cdots > k_{r} \\ k_{r+1} > \cdots > k_{r+s}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{r+s}})^{n_{r+s}}}}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}} \\ & = \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r} \\ k_{r+1} > \cdots > k_{r+s}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{r+1}})}}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}}} \\ & + \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r} \\ k_{r+1} > \cdots > k_{r+s}}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{1}})}}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}}} \\ & + \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r+s} \\ k_{r+1} > \cdots > k_{r+s}}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{1}})}}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}}} \\ & + \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r+s} \\ k_{r+1} > \cdots > k_{r+s}}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{1}})}}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}}} \\ & + \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r+s} \\ k_{r+1} > \cdots > k_{r+s}}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{1}})}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}}} \\ & + \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r+s} \\ k_{r+1} > \cdots > k_{r+s}}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{1}})}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}}} \\ & + \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r+s} \\ k_{r+1} > \cdots > k_{r+s}}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{1}})}{(1 - q^{k_{1}})^{n_{1}} \cdots (1 - q^{k_{r+s}})^{n_{r+s}}} \\ & + \sum_{\substack{k_{1} < k_{r+1}, k_{1} > \cdots > k_{r+s} \\ k_{r+1} > \cdots > k_{r+s}}}} \frac{q^{k_{1}} - q^{k_{1}} (1 - q^{k_{1}})}{(1 - q^{k$$

which proves the claim.

**4.6.** The differential algebra structure. We introduce the derivation  $\delta := q(d/dq)$ .

Proposition 4.6. For any  $a_1, \ldots, a_k \in \mathbb{Z}^k$ ,

$$\delta_{\bar{3}q}(a_1, \dots, a_k) = \left(k - \sum_{r=1}^k a_r(k - r + 1)\right)_{\bar{3}q}(a_1, \dots, a_k)$$

$$+ \sum_{r=1}^k a_r(k - r + 1)_{\bar{3}q}(a_1, \dots, a_r + 1, \dots, a_k)$$

$$+ \sum_{s=1}^k \left(1 - \sum_{r=1}^s a_r\right)_{\bar{3}q}(a_1, \dots, a_s, 0, a_{s+1}, \dots, a_k)$$

$$+ \sum_{1 \le r \le s \le k} a_r \bar{3}_q(a_1, \dots, a_r + 1, \dots, a_s, 0, a_{s+1}, \dots, a_k).$$

Proof. By a straightforward computation,

$$\begin{split} \delta \overline{\mathfrak{z}}_{q}(a_{1},\ldots,a_{k}) &= \sum_{m_{1}>\cdots>m_{k}>0} \delta \frac{q^{m_{1}}}{(1-q^{m_{1}})^{a_{1}}\cdots(1-q^{m_{k}})^{a_{k}}} \\ &= \sum_{m_{1}>\cdots>m_{k}>0} \frac{m_{1}q^{m_{1}}}{(1-q^{m_{1}})^{a_{1}}\cdots(1-q^{m_{k}})^{a_{k}}} \\ &+ \sum_{m_{1}>\cdots>m_{k}>0} \sum_{r=1}^{k} \frac{a_{r}m_{r}q^{m_{1}+m_{r}}}{(1-q^{m_{1}})^{a_{1}}\cdots(1-q^{m_{r}})^{a_{r}+1}\cdots(1-q^{m_{k}})^{a_{k}}} \\ &= \sum_{m_{1}>\cdots>m_{k}>0} \frac{m_{1}q^{m_{1}}}{(1-q^{m_{1}})^{a_{1}}\cdots(1-q^{m_{k}})^{a_{k}}} \\ &+ \sum_{m_{1}>\cdots>m_{k}>0} \sum_{r=1}^{k} \frac{a_{r}m_{r}q^{m_{1}}-a_{r}m_{r}q^{m_{1}}(1-q^{m_{r}})}{(1-q^{m_{1}})^{a_{1}}\cdots(1-q^{m_{r}})^{a_{r}+1}\cdots(1-q^{m_{k}})^{a_{k}}}. \end{split}$$

Decomposing the integers  $m_r$  as

$$m_r = (k - r + 1) + (m_r - m_{r+1} - 1) + \dots + (m_{k-1} - m_k - 1) + (m_k - 1)$$

then gives the desired result.

Proposition 4.6 in depth one then gives the following result.

Corollary 4.7. For any  $a \in \mathbb{Z}$ ,

$$\delta \bar{\mathfrak{z}}_a(a) = (1-a)(\bar{\mathfrak{z}}_a(a,0) + \bar{\mathfrak{z}}_a(a)) + a(\bar{\mathfrak{z}}_a(a+1,0) + \bar{\mathfrak{z}}_a(a+1)).$$

#### 5. Double *q*-shuffle relations

**5.1. Double q-shuffle relations for modified qMZVs.** We can define a bijective map that changes the letter  $z_n$  into the word  $p^n y$ :

$$\mathfrak{r}: \widetilde{Y}^* \stackrel{\sim}{\longrightarrow} W$$

$$z_{n_1} \cdots z_{n_k} \longmapsto p^{n_1} y \cdots p^{n_k} y.$$

We have seen above that  $\bar{\mathfrak{z}}_q(n_1,\ldots,n_k) = \bar{\mathfrak{z}}_q^{\text{III}}(p^{n_1}y\cdots p^{n_k}y) = \bar{\mathfrak{z}}_q^{\text{III}}(z_{n_1}\cdots z_{n_k})$ . From this, we obtain  $\bar{\mathfrak{z}}_q^{\text{III}} = \bar{\mathfrak{z}}_q^{\text{III}} \circ \mathfrak{r}$  and the double *q*-shuffle relations

$$\bar{\mathfrak{z}}_{q}^{\text{III}}(u)\bar{\mathfrak{z}}_{q}^{\text{III}}(v) = \bar{\mathfrak{z}}_{q}^{\text{III}}(u \coprod v), \quad \bar{\mathfrak{z}}_{q}^{\text{IH}}(u')\bar{\mathfrak{z}}_{q}^{\text{IH}}(v') = \bar{\mathfrak{z}}_{q}^{\text{IH}}(u' \coprod v') \tag{5.1}$$

for any words  $u, v \in W$ , respectively,  $u', v' \in \widetilde{Y}^*$ . From (5.1), we immediately deduce that

$$\bar{\mathfrak{z}}_q^{\text{III}}(\mathfrak{r}(u') \coprod \mathfrak{r}(v') - \mathfrak{r}(u' \coprod v')) = 0 \tag{5.2}$$

for any  $u', v' \in \widetilde{Y}^*$  or, alternatively,

$$\overline{\mathfrak{z}}_q^{\scriptscriptstyle{\mathsf{H}}\mathsf{I}}\left(\mathfrak{r}^{-1}(u) \coprod \mathfrak{r}^{-1}(v) - \mathfrak{r}^{-1}(u \coprod v)\right) = 0$$

for any  $u, v \in W$ .

**5.2. Double q-shuffle relations for nonmodified qMZVs.** We introduce a natural notion of weight for words<sup>1</sup> in both  $\widetilde{Y}^*$  and W, which takes integer values of any sign:

$$w(z_{n_1}\cdots z_{n_k})=w(p^{n_1}y\cdots p^{n_k}y):=n_1+\cdots+n_k.$$

Let us denote by  $\mathcal{Y}$  (respectively W) the  $\mathbb{Q}$ -vector space spanned by  $\widetilde{Y}^*$  (respectively W) endowed with the product  $\mathbb{H}$  (respectively  $\mathbb{H}$ ). Both products are filtered, but not graded, with respect to the weight: if  $\mathcal{Y}^{(n)}$  (respectively  $W^{(n)}$ ) stands for the linear span of words in  $\widetilde{Y}^*$  (respectively W) of weight  $\leq n$ ,

$$\mathcal{Y}^{(n)} \coprod \mathcal{Y}^{(m)} \subset \mathcal{Y}^{(n+m)}$$
 and  $\mathcal{W}^{(n)} \coprod \mathcal{W}^{(m)} \subset \mathcal{W}^{(n+m)}$ .

A graded version can be introduced as follows: introduce the Laurent polynomials in the indeterminate h with coefficients in  $\mathcal{Y}$  (respectively  $\mathcal{W}$ ) and give weight 1 to h. The swap r is linearly extended to a linear isomorphism from  $\mathcal{Y}$  onto  $\mathcal{W}$  and then from  $\mathcal{Y}[h^{-1},h]$  onto  $\mathcal{W}[h^{-1},h]$  by extension of scalars. The products  $\mathcal{Y}$  and  $\mathcal{Y}$  is extended  $\mathcal{Y}$  and  $\mathcal{Y}$ , respectively. The letter  $\mathcal{Y}$  will stand here for 1-h, for reasons which will become clear in the sequel. Consider the linear transformation

$$H_q: \mathcal{Y}[h^{-1}, h] \longrightarrow \mathcal{Y}[h^{-1}, h]$$
  
 $u' \longmapsto h^{w(u')}u'$ 

and consider the analogous map on  $W[h^{-1}, h]$ , which will also be called  $H_q$ . Let us now introduce two products  $\coprod_q$  and  $\coprod_q$  on  $\mathcal{Y}[h^{-1}, h]$  and  $W[h^{-1}, h]$ , respectively, by

$$u' \coprod_q v' := H_q^{-1}(H_qu' \coprod H_qv') \quad \text{and} \quad u \coprod_q v := H_q^{-1}(H_qu \coprod H_qv).$$

We *h*-bilinearly extend the maps  $\mathfrak{z}_q^{\text{IM}}$  and  $\mathfrak{z}_q^{\text{III}}$  to the Laurent polynomials by sending *h* to 1-q. We can now display the double *q*-shuffle relations for nonmodified *qMZVs*.

Proposition 5.1.

$$\mathfrak{z}_q^{\mathrm{IH}} = \mathfrak{z}_q^{\mathrm{III}} \circ \mathfrak{r}, \qquad \mathfrak{z}_q^{\mathrm{III}}(u) \mathfrak{z}_q^{\mathrm{III}}(v) = \mathfrak{z}_q^{\mathrm{III}}(u \coprod_q v) \quad \text{and} \quad \mathfrak{z}_q^{\mathrm{IH}}(u') \mathfrak{z}_q^{\mathrm{IH}}(v') = \mathfrak{z}_q^{\mathrm{IH}}(u' \coprod_q v').$$

**PROOF.** This is immediate from (4.2), (5.1) and the definitions of the two new products.

Note that the two new products are now graded (with respect to the weight) and

$$(yv) \coprod_q u = v \coprod_q (yu) = y(v \coprod_q u),$$
 
$$pv \coprod_q pu = p(v \coprod_q pu) + p(pv \coprod_q u) - hp(v \coprod_q u),$$
 
$$hdv \coprod_q du = v \coprod_q du + dv \coprod_q u - d(v \coprod_q u),$$
 
$$dv \coprod_q pu = pu \coprod_q dv = d(v \coprod_q pu) - v \coprod_q u + hdv \coprod_q u,$$

as well as

$$u' \coprod_{a} v' = T_a^{-1}(T_a u' * T_a v'),$$
 (5.3)

<sup>&</sup>lt;sup>1</sup>This should not cause confusion with the notion of weight for a Rota–Baxter operator introduced before.

where the operator  $T_q$  is defined by

$$T_q(z_nv') := (z_n - hz_{n-1})v'$$

for any  $n \in \mathbb{Z}$  and for any  $v' \in \widetilde{Y}^*$ . Strictly speaking, the operator  $T_q^{-1}$  is defined on the space  $\mathcal{Y}[h^{-1}, h]$  of Laurent series with coefficients in  $\mathcal{Y}$  by the series

$$T_q^{-1}(z_n v') = \sum_{k \ge 0} h^k z_{n-k} v',$$

but it does not show up in the expression of the product  $\mathbb{H}_q$  in terms of the ordinary quasi-shuffle product \*. Indeed, (5.3) yields

$$z_m u' \coprod_q z_n v' = z_m (u' * T_q(z_n v')) + z_n (T_q(z_m u') * v') + T_q(z_{m+n}(u' * v')).$$

Finally, any Laurent polynomial in h can be seen as a formal series in q. All results in this paragraph, except the grading, still hold over the ring  $\mathbb{Q}[[q]]$  with h = 1 - q.

**5.3. Digression on Schlesinger** q**-MZVs.** The Schlesinger MZVs are defined as follows:

$$\mathfrak{z}_{q}^{S}(n_{1},\ldots,n_{k}) = (1-q)^{w} \underbrace{P\left[P\left[\cdots P\left[\bar{y}\cdots P\left[\bar{y}\cdots P\left[P\left[\cdots P\left[\bar{y}\right]\right]\right]\right]\right]\cdots\right]\right]}_{n_{1}}(1)$$

$$= \sum_{m_{1}>\cdots>m_{k}>0} \frac{1}{[m_{1}]_{q}^{n_{1}}\cdots[m_{k}]_{q}^{n_{k}}}.$$

They are defined for |q| > 1 for  $n_j \ge 1$  and  $n_1 \ge 2$ , and converge to the corresponding classical MZVs as  $q \to 1$  (by the monotone convergence theorem). A straightforward computation yields

$$\mathfrak{z}_q^S(n_1,\ldots,n_k) = \sum_{m_1 > \cdots > m_k > 0} \frac{(q^{-1})^{(m_1-1)n_1 + \cdots + (m_k-1)n_k}}{[m_1]_{q^{-1}}^{n_1} \cdots [m_k]_{q^{-1}}^{n_k}}.$$

In other words,  $\mathfrak{F}_q^S(n_1,\ldots,n_k) = \mathfrak{F}_{q^{-1}}^B(n_1,\ldots,n_k)$ , where the superscript B stands for the Bradley model (see [4] and [6]). Hence,  $\mathfrak{F}_q^S(n_1,\ldots,n_k)$  also makes sense as a formal series in  $q^{-1}$  for  $n_i \geq 0$  and  $n_1 \geq 1$ . Now let us introduce the following notation:

$$\begin{split} \widetilde{Y}_1^* &:= \{z_{n_1} \cdots z_{n_k} \in \widetilde{Y}^*, \ n_j \geq 1\}, \\ \widetilde{Y}_2^* &:= \{z_{n_1} \cdots z_{n_k} \in \widetilde{Y}^*, \ n_j \geq 1 \ \text{and} \ n_1 \geq 2\}, \\ \mathcal{Y}_1 &:= \mathbb{Q}\text{-linear span of} \ \widetilde{Y}_1^*, \\ \mathcal{Y}_2 &:= \mathbb{Q}\text{-linear span of} \ \widetilde{Y}_2^*, \\ \mathfrak{z}_q^{S \text{ int}} \ (z_{n_1} \cdots z_{n_k}) &:= \mathfrak{z}_q^S (n_1, \dots, n_k), \qquad z_{n_1} \cdots z_{n_k} \in \widetilde{Y}_1^*. \end{split}$$

Proposition 5.2. The following diagram commutes:

$$\begin{array}{c} \mathcal{Y}_{1}[[q^{-1}]] \\ \uparrow^{T_{q}} \\ \downarrow^{T_{q}} \\ q^{-1}\mathcal{Y}_{2}[[q^{-1}]] \\ \xrightarrow{\delta_{q}^{\mathbf{IH}}} \\ \end{array} \rightarrow \mathbb{Q}[[q^{-1}]]$$

**PROOF.** This is a straightforward formal computation using the equality  $1 - (1 - q)[m_1]_q = q^{m_1}$ .

**5.4.** q-Analogue of regularised double q-shuffle relations. In the following, we restrict to nonnegative indices. Thanks to the q-regularisation, we observe that the double q-shuffle relation yields

$$\bar{\mathfrak{z}}_{q}(1)\bar{\mathfrak{z}}_{q}(2) = \bar{\mathfrak{z}}_{q}(1,2) + \bar{\mathfrak{z}}_{q}(2,1) + \bar{\mathfrak{z}}_{q}(3) - \bar{\mathfrak{z}}_{q}(1,1) - \bar{\mathfrak{z}}_{q}(2,0) - \bar{\mathfrak{z}}_{q}(2) 
= \bar{\mathfrak{z}}_{q}(1,2) + 2\bar{\mathfrak{z}}_{q}(2,1) - \bar{\mathfrak{z}}_{q}(2,0) - \bar{\mathfrak{z}}_{q}(1,1),$$

from which we obtain the relation

$$\bar{\mathfrak{z}}_q(3) - \bar{\mathfrak{z}}_q(2) = \bar{\mathfrak{z}}_q(2,1).$$
 (5.4)

For the proper qMZVs defined in (4.1), this gives

$$\mathfrak{z}_q(3) - (1-q)\mathfrak{z}_q(2) = \mathfrak{z}_q(2,1),$$

which, in the limit  $q \to 1$ , reduces to the classical relation  $\zeta(2, 1) = \zeta(3)$  (see (1.5) above). Equation (5.4) is equivalent to an algebraic identity established by E. T. Bell in the 1930s (see [3], page 158).<sup>1</sup>

We denote by  $\mathbb{Q}.\widetilde{Y}_{\text{conv}}^*$  the free associative algebra generated by the set of words  $\widetilde{Y}_{\text{conv}}^*$ , the submonoid of words  $z_{n_1}\cdots z_{n_k}$  with letters in  $\widetilde{Y}_+:=\{z_n,\ n\in\mathbb{N}\}$  and  $n_1>1$ . We arrive at a q-analogue of Hoffman's regularisation relations. By virtue of the q-regularisation, this is a particular case of (5.2).

Proposition 5.3. For any  $v \in \mathbb{Q}.\widetilde{Y}_{\text{conv}}^*$ 

$$\bar{\mathfrak{z}}_q^{\mathrm{III}}(py \coprod \mathfrak{r}(v) - \mathfrak{r}(z_1 \coprod v)) = 0,$$

respectively,

$$g_a^{\text{III}}(py \coprod r(v) - r(z_1 \coprod v)) = 0.$$
 (5.5)

Since terms of depth smaller than |v| + 1 disappear in the limit  $q \to 1$ , identity (5.5) reduces to Hoffman's regularisation relations (2.3) for MZVs.

As there are no regularisation issues involved, no correction analogous to  $\rho$  (in the notation of Section 2) is needed to go from the q-quasi-shuffle picture to the q-shuffle picture or *vice versa*. It would be interesting to understand in detail how the correction map  $\rho$  surfaces when  $q \to 1$ .

<sup>&</sup>lt;sup>1</sup>We thank W. Zudilin for kindly drawing our attention to reference [3].

### Acknowledgements

We thank W. Zudilin for his most valuable comments and encouragement, as well as H. Bachmann and U. Kühn for illuminating discussions. We also thank J. Singer and J. Zhao for comments and remarks.

#### References

- [1] L. V. Ahlfors, Complex Analysis, 3rd edn (McGraw-Hill Higher Education, New York, 1980).
- [2] H. Bachmann and U. Kühn, 'The algebra of multiple divisor functions and applications to multiple zeta values', arXiv:1309.3920.
- [3] W. N. Bailey, 'An algebraic identity', J. Lond. Math. Soc. 11 (1936), 156–160.
- [4] D. M. Bradley, 'Multiple *q*-zeta values', *J. Algebra* **283** (2005), 752–798.
- [5] P. Cartier, 'Fonctions polylogarithmes, nombres polyzêtas et groupes prounipotents', Sémin. Bourbaki 885 (2001), 137–173.
- [6] J. Castillo Medina, K. Ebrahimi-Fard and D. Manchon, 'On Euler's decomposition formula for q-MZVs', Ramanujan J. to appear; doi:10.1007/s11139-014-9638-8.
- [7] J. Castillo Medina, K. Ebrahimi-Fard and D. Manchon, 'Unfolding the double shuffle structure of q-MZVs', arXiv:1310.1330.
- [8] I. Cherednik, 'On q-analogues of Riemann's zeta function', Selecta Math. (N.S.) 7(4) (2001), 447–491.
- [9] R. Díaz and M. Páez, 'An identity in Rota-Baxter algebras', Sém. Lothar. Combin. 57 (2007), B57b, 8 pages.
- [10] K. Ebrahimi-Fard and F. Patras, 'La structure combinatoire du calcul intégral', Gaz. Math. 138 (2013), 5–22. Société Mathématique de France (SMF). English translation: 'Rota–Baxter algebra. The combinatorial structure of integral calculus', arXiv:1304.1204v1.
- [11] L. Guo and W. Keigher, 'On differential Rota–Baxter algebras', J. Pure Appl. Algebra 212 (2008), 522–540.
- [12] M. E. Hoffman, 'The algebra of multiple harmonic series', J. Algebra 194(2) (1997), 477–495.
- [13] M. E. Hoffman, 'Quasi-shuffle products', J. Algebraic Combin. 11 (2000), 49–68.
- [14] M. E. Hoffman, 'Algebraic aspects of multiple zeta values', in: Zeta Functions, Topology and Quantum Physics (eds. T. Aoki et al.) (Springer, New York, 2005), 51–74.
- [15] K. Ihara, M. Kaneko and D. Zagier, 'Derivation and double shuffle relations for multiple zeta values', Compositio Math. 142 (2006), 307–338.
- [16] M. Kaneko, N. Kurokawa and M. Wakayama, 'A variation of Euler's approach to values of the Riemann zeta function', Kyushu J. Math. 57 (2003), 175–192.
- [17] Y. Ohno, J. Okuda and W. Zudilin, 'Cyclic q-MZSV sum', J. Number Theory 132 (2012), 144–155.
- [18] A. Okounkov, 'Hilbert schemes and multiple *q*-zeta values', *Funct. Anal. Appl.* **48**(2) (2014), 138–144.
- [19] G. Racinet, 'Doubles mélanges des polylogarithmes multiples aux racines de l'unité', Publ. Math. Inst. Hautes Études Sci. 95 (2002), 185–231.
- [20] G.-C. Rota, 'Baxter operators, an introduction', in: Gian-Carlo Rota on Combinatorics: Introductory Papers and Commentaries, Contemporary Mathematicians (ed. J. P. S. Kung) (Birkhäuser, Boston, MA, 1995).
- [21] G.-C. Rota and D. A. Smith, 'Fluctuation theory and Baxter algebras', Symp. Math. IX (1971), 179–201.
- [22] K. G. Schlesinger, 'Some remarks on *q*-deformed multiple polylogarithms', Preprint, arXiv:math/0111022, 2001.
- [23] Y. Takeyama, 'The algebra of a q-analogue of multiple harmonic series', Symmetry Integrability Geom. Methods Appl. 9 (2013), 061.
- [24] M. Waldschmidt, 'Valeurs, zêta multiples: une introduction', J. Théor. Nombres Bordeaux 12 (2000), 581–595.

- [25] M. Waldschmidt, 'Multiple polylogarithms', Lecture at Institute of Mathematical Sciences, Chennai, November 2000, available at http://www.math.jussieu.fr/ miw/articles/.
- [26] D. Zagier, 'Values of zeta functions and their applications', in: First European Congress of Mathematics, Progress in Mathematics, 120, Vol. II (Birkhäuser, Basel, 1994), 497–512.
- [27] J. Zhao, 'q-Multiple zeta functions and q-multiple polylogarithms', Ramanujan J. 14 (2007), 189–221.
- [28] W. Zudilin, 'Algebraic relations for multiple zeta values', *Russian Math. Surveys* **58**(1) (2003), 1–29.

JAIME CASTILLO-MEDINA, Universidad de València, Facultat de Ciències Matemàtiques, C/-Doctor Moliner, 50, 46100 Burjassot-Valencia, Spain e-mail: jaicasme@alumni.uv.es

KURUSCH EBRAHIMI-FARD, Instituto de Ciencias Matemáticas, C/-Nicolás Cabrera, no. 13–15, 28049 Madrid, Spain e-mail: kurusch@icmat.es, kurusch.ebrahimi-fard@uha.fr

DOMINIQUE MANCHON, Université Blaise Pascal, CNRS-UMR 6620, 63177 Aubière, France

e-mail: manchon@math.univ-bpclermont.fr