

## On multiple L-values

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## On multiple $L$ -values

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**Abstract.** We formulate and prove regularized double shuffle and derivation relations for multiple  $L$ -values. A description of principal part of a multiple  $L$ -function is also given.

### 0. Introduction.

In the present paper, we study the regularized double shuffle and the derivation relations of the multiple  $L$ -values and give some applications. A fair amount of work related to the multiple  $L$ -values has already been done, *e.g.*, A. Goncharov [G1], [G2], G. Racinet [R] and the references therein. In particular, the regularization stuff is also treated in a series of works of Goncharov and Racinet. Our approach here, which largely follows the setup and method given in [IKZ] for multiple zeta values, is less abstract and more directly aimed at obtaining relations among multiple  $L$ -values. In particular, a generalization of the derivation relation of multiple zeta values, which as shown in [IKZ] is in a sense equivalent to the regularized double shuffle relation, is established by using the regularization and the method developed in [IKZ].

In §1 we present some basic definitions and algebraic setup introduced by M. Hoffman [H] which is suitable for our study. In §2, after the discussion on the finite double shuffle relation (Proposition 2.1), we give the regularized double shuffle relations (Theorem 2.3, Theorem 2.4). The derivation relation (Theorem 3.1) is formulated and proved in §3. The final §4 is devoted to a couple of applications of the results and ideas developed in the previous sections. Of them, the principal part of a certain multiple  $L$ -function is determined (Theorem 4.1) in terms of the polynomials defined algebraically to describe the regularization procedure.

### 1. Definition and algebraic setup.

#### 1.1. Definition.

We define two types of multiple  $L$ -values in a general context. Let  $m$  be a natural number and  $R = R_m$  denote the  $\mathbf{Z}$ -module  $\mathbf{Z}/m\mathbf{Z}$ . Let  $\mathcal{F}(R; \mathbf{C})$  be the  $\mathbf{C}$ -vector space consisting of all mappings  $f : R \rightarrow \mathbf{C}$ . An element  $f \in \mathcal{F}(R; \mathbf{C})$  is viewed naturally as a function on  $\mathbf{Z}$  via the projection  $\mathbf{Z} \rightarrow R$ . We fix once and for all a primitive  $m$ th root of unity  $\zeta = \zeta_m := \exp(2\pi i/m)$ . For each  $a \in R$ , let  $\varphi_a \in \mathcal{F}(R; \mathbf{C})$  be defined by

$$\varphi_a(x) = \zeta^{ax} \quad (x \in R).$$

The set of functions  $\{\varphi_a\}_{a \in R}$  constitute a basis of the space  $\mathcal{F}(R; \mathbf{C})$ . The expression of an element  $f \in \mathcal{F}(R; \mathbf{C})$  by this basis is the Fourier expansion of  $f$ :

$$(1) \quad f(x) = \sum_{a \in R} \hat{f}(a) \zeta^{ax} \quad \text{with} \quad \hat{f}(a) = \frac{1}{m} \sum_{y \in R} f(y) \zeta^{-ay},$$

the function  $\hat{f}$  being referred to as the (finite) Fourier transform of  $f$ .

For  $f_1, \dots, f_n \in \mathcal{F}(R; \mathbf{C})$  and positive integers  $k_1, \dots, k_n$ , we define the multiple  $L$ -values  $L_{\square}(k_1, \dots, k_n; f_1, \dots, f_n)$  and  $L_*(k_1, \dots, k_n; f_1, \dots, f_n)$  by

$$(2) \quad \begin{aligned} & L_{\square}(k_1, \dots, k_n; f_1, \dots, f_n) \\ &= \sum_{m_1 > m_2 > \dots > m_n > 0} \frac{f_1(m_1 - m_2) \cdots f_{n-1}(m_{n-1} - m_n) f_n(m_n)}{m_1^{k_1} m_2^{k_2} \cdots m_n^{k_n}} \\ &= \sum_{\mu_1=1}^{\infty} \cdots \sum_{\mu_n=1}^{\infty} \frac{f_1(\mu_1) f_2(\mu_2) \cdots f_n(\mu_n)}{(\mu_1 + \cdots + \mu_n)^{k_1} (\mu_2 + \cdots + \mu_n)^{k_2} \cdots (\mu_n)^{k_n}} \end{aligned}$$

and

$$(3) \quad \begin{aligned} & L_*(k_1, \dots, k_n; f_1, \dots, f_n) \\ &= \sum_{m_1 > m_2 > \dots > m_n > 0} \frac{f_1(m_1) f_2(m_2) \cdots f_n(m_n)}{m_1^{k_1} m_2^{k_2} \cdots m_n^{k_n}} \\ &= \sum_{\mu_1=1}^{\infty} \cdots \sum_{\mu_n=1}^{\infty} \frac{f_1(\mu_1 + \cdots + \mu_n) f_2(\mu_2 + \cdots + \mu_n) \cdots f_n(\mu_n)}{(\mu_1 + \cdots + \mu_n)^{k_1} (\mu_2 + \cdots + \mu_n)^{k_2} \cdots (\mu_n)^{k_n}}. \end{aligned}$$

If  $n = 1$ , the two series coincide. When  $k_1 \geq 2$ , these infinite series are absolutely convergent. When  $k_1 = 1$ , the series are understood to be the limits

$$\begin{aligned} & L_{\square}(1, k_2, \dots, k_n; f_1, \dots, f_n) \\ &= \lim_{R \rightarrow \infty} \sum_{R \geq m_1 > m_2 > \dots > m_n > 0} \frac{f_1(m_1 - m_2) f_2(m_2 - m_3) \cdots f_{n-1}(m_{n-1} - m_n) f_n(m_n)}{m_1 m_2^{k_2} \cdots m_n^{k_n}}, \\ & L_*(1, k_2, \dots, k_n; f_1, \dots, f_n) \\ &= \lim_{R \rightarrow \infty} \sum_{R \geq m_1 > m_2 > \dots > m_n > 0} \frac{f_1(m_1) f_2(m_2) \cdots f_n(m_n)}{m_1 m_2^{k_2} \cdots m_n^{k_n}}, \end{aligned}$$

provided they are convergent. As for the convergence, we have the following criterion.

**PROPOSITION 1.1.** *Suppose  $k_1 = 1$ . The series  $L_{\square}(1, k_2, \dots, k_n; f_1, \dots, f_n)$  and  $L_*(1, k_2, \dots, k_n; f_1, \dots, f_n)$  are convergent if and only if  $\hat{f}_1(0) = 0$ , (i.e.,  $\sum_{y \in R} f_1(y) = 0$ ).*

**PROOF.** We give a proof based on the standard method of Abel's summation for  $L_{\square}$ . The other case is similar or can be deduced from this using the next proposition. Put  $S(n) := \sum_{m=1}^n f_1(m)$ ,  $S(0) = 0$ , and

$$L(R) := \sum_{R \geq m_1 > m_2 > \dots > m_n > 0} \frac{f_1(\mu_1) f_2(\mu_2) \cdots f_n(\mu_n)}{m_1 m_2^{k_2} \cdots m_n^{k_n}}$$

where  $\mu_1 = m_1 - m_2$ ,  $\mu_2 = m_2 - m_3, \dots, \mu_n = m_n$ . By the relation  $f_1(\mu_1) = S(\mu_1) - S(\mu_1 - 1)$ , we have

$$\begin{aligned} L(R) &= \sum_{R \geq m_1 > m_2 > \dots > m_n > 0} \frac{(S(\mu_1) - S(\mu_1 - 1))f_2(\mu_2) \cdots f_n(\mu_n)}{m_1 m_2^{k_2} \cdots m_n^{k_n}} \\ &= \sum_{\substack{R \geq \mu_1 + \mu_2 + \dots + \mu_n \\ \mu_j \geq 1}} \frac{S(\mu_1)f_2(\mu_2) \cdots f_n(\mu_n)}{(\mu_1 + \mu_2 + \dots + \mu_n)(\mu_2 + \dots + \mu_n)^{k_2} \cdots \mu_n^{k_n}} \\ &\quad - \sum_{\substack{R \geq \mu'_1 + 1 + \mu_2 + \dots + \mu_n \\ \mu'_1 \geq 0, \mu_j \geq 1 \ (j \geq 2)}} \frac{S(\mu'_1)f_2(\mu_2) \cdots f_n(\mu_n)}{(\mu'_1 + 1 + \mu_2 + \dots + \mu_n)(\mu_2 + \dots + \mu_n)^{k_2} \cdots \mu_n^{k_n}} \quad (\mu'_1 = \mu_1 - 1). \end{aligned}$$

Noting  $S(0) = 0$  and dividing the first sum into two parts according as  $R = \mu_1 + \mu_2 + \dots + \mu_n$  and  $R \geq \mu_1 + \mu_2 + \dots + \mu_n + 1$ , we find

$$\begin{aligned} L(R) &= \sum_{\substack{R = \mu_1 + \mu_2 + \dots + \mu_n \\ \mu_j \geq 1}} \frac{S(\mu_1)f_2(\mu_2) \cdots f_n(\mu_n)}{(\mu_1 + \mu_2 + \dots + \mu_n)(\mu_2 + \dots + \mu_n)^{k_2} \cdots \mu_n^{k_n}} \\ &\quad + \sum_{\substack{R \geq \mu_1 + \mu_2 + \dots + \mu_n + 1 \\ \mu_j \geq 1}} \frac{S(\mu_1)f_2(\mu_2) \cdots f_n(\mu_n)}{(\mu_2 + \dots + \mu_n)^{k_2} \cdots \mu_n^{k_n}} \\ &\quad \times \left( \frac{1}{\mu_1 + \mu_2 + \dots + \mu_n} - \frac{1}{\mu_1 + \mu_2 + \dots + \mu_n + 1} \right). \end{aligned}$$

By the assumption  $\hat{f}_1(0) = 0$ , the sum  $S(n)$  is periodic and so bounded, hence there is a constant  $M > 0$  such that

$$|S(n)| \leq M, \quad |f_j(n)| \leq M \quad (\forall n, j).$$

From this and

$$\frac{1}{\mu_1 + \mu_2 + \dots + \mu_n} - \frac{1}{\mu_1 + \mu_2 + \dots + \mu_n + 1} \leq \frac{1}{(\mu_1 + \mu_2 + \dots + \mu_n)^2},$$

we have the estimate

$$\begin{aligned} |L(R)| &\leq \sum_{\substack{R = \mu_1 + \mu_2 + \dots + \mu_n \\ \mu_j \geq 1}} \frac{M^n}{(\mu_1 + \mu_2 + \dots + \mu_n)(\mu_2 + \dots + \mu_n)^{k_2} \cdots \mu_n^{k_n}} \\ &\quad + \sum_{\substack{R-1 \geq \mu_1 + \mu_2 + \dots + \mu_n \\ \mu_j \geq 1}} \frac{M^n}{(\mu_1 + \mu_2 + \dots + \mu_n)^2 (\mu_2 + \dots + \mu_n)^{k_2} \cdots \mu_n^{k_n}} \\ &\leq \sum_{\substack{R-1 \geq \mu_2 + \dots + \mu_n \\ \mu_j \geq 1}} \frac{M^n}{(\mu_2 + \dots + \mu_n)^{k_2+1} \cdots \mu_n^{k_n}} \\ &\quad + \sum_{\substack{R-1 \geq \mu_1 + \mu_2 + \dots + \mu_n \\ \mu_j \geq 1}} \frac{M^n}{(\mu_1 + \mu_2 + \dots + \mu_n)^2 (\mu_2 + \dots + \mu_n)^{k_2} \cdots \mu_n^{k_n}}. \end{aligned}$$

Both sums on the right converge as  $R \rightarrow \infty$  and so  $L(R)$  converges. If  $\hat{f}_1(0) \neq 0$ , then  $S(n)$  is unbounded and the sum  $L(R)$  obviously diverges.  $\square$

From here on until we consider the regularization of divergent series, we always assume  $\hat{f}_1(0) = 0$  if  $k_1 = 1$ .

Each of the two types of MLV's (2) and (3) is expressed as a linear combination of the other type of MLV's.

PROPOSITION 1.2. *We have*

$$\begin{aligned} L_*(k_1, \dots, k_n; f_1, \dots, f_n) \\ = \sum_{a_1, \dots, a_n \in R} \hat{f}_1(a_1) \cdots \hat{f}_n(a_n) L_{\mathfrak{W}}(k_1, \dots, k_n; \varphi_{a_1}, \varphi_{a_1+a_2}, \dots, \varphi_{a_1+\dots+a_n}) \end{aligned}$$

and

$$\begin{aligned} L_{\mathfrak{W}}(k_1, \dots, k_n; f_1, \dots, f_n) \\ = \sum_{a_1, \dots, a_n \in R} \hat{f}_1(a_1) \cdots \hat{f}_n(a_n) L_*(k_1, \dots, k_n; \varphi_{a_1}, \varphi_{a_2-a_1}, \dots, \varphi_{a_n-a_{n-1}}). \end{aligned}$$

In particular, for  $a_1, \dots, a_n \in R$  with  $a_1 \neq 0$ , we have

$$\begin{aligned} (4) \quad L_*(k_1, \dots, k_n; \varphi_{a_1}, \dots, \varphi_{a_n}) &= L_{\mathfrak{W}}(k_1, \dots, k_n; \varphi_{a_1}, \varphi_{a_1+a_2}, \dots, \varphi_{a_1+\dots+a_n}), \\ L_{\mathfrak{W}}(k_1, \dots, k_n; \varphi_{a_1}, \dots, \varphi_{a_n}) &= L_*(k_1, \dots, k_n; \varphi_{a_1}, \varphi_{a_2-a_1}, \dots, \varphi_{a_n-a_{n-1}}). \end{aligned}$$

PROOF. This is an immediate consequence of (1), the special case being obtained by setting  $f_j = \varphi_{a_j}$  and noting  $\hat{\varphi}_a(x) = 1$  for  $x = a$  and 0 otherwise.  $\square$

For the sake of simplicity we write  $L_{\#}(k_1, \dots, k_n; a_1, \dots, a_n)$  or  $L_{\#}(\mathbf{k}; \mathbf{a})$  with  $(\mathbf{k}; \mathbf{a}) = (k_1, \dots, k_n; a_1, \dots, a_n)$  for  $L_{\#}(k_1, \dots, k_n; \varphi_{a_1}, \dots, \varphi_{a_n})$  ( $\# = \mathfrak{W}$  or  $*$ ). The index set  $(\mathbf{k}; \mathbf{a}) = (k_1, \dots, k_n; a_1, \dots, a_n)$  for which the series  $L_{\#}(\mathbf{k}; \mathbf{a})$  is convergent is called *admissible*. This is the case when  $k_1 \geq 2$ , or  $k_1 = 1$  and  $a_1 \neq 0$  in  $R_m$  as Proposition (1.1) shows. We also note that if  $a_1 = \dots = a_n = 0$  in  $R_m$  both of our MLV's coincide with the multiple zeta value and the index set is admissible if and only if  $k_1 \geq 2$ :

$$L_{\mathfrak{W}}(k_1, \dots, k_n; 0, \dots, 0) = L_*(k_1, \dots, k_n; 0, \dots, 0) = \zeta(k_1, \dots, k_n).$$

In the theory of multiple zeta values, the iterated integral expression (the Drinfeld integral) played an important role. The series  $L_{\mathfrak{W}}(k_1, \dots, k_n; a_1, \dots, a_n)$  has a similar integral expression as follows. Let

$$I(\varepsilon_1, \dots, \varepsilon_k) = \int \cdots \int_{1 > t_1 > \cdots > t_k > 0} A_{\varepsilon_1}(t_1) A_{\varepsilon_2}(t_2) \cdots A_{\varepsilon_k}(t_k) dt_1 \cdots dt_k,$$

where  $\varepsilon_j$  ( $1 \leq j \leq k$ ) are complex numbers with  $|\varepsilon_j| \leq 1$  and

$$A_0(t) = \frac{1}{t} \quad \text{and} \quad A_{\varepsilon}(t) = \frac{\varepsilon}{1 - \varepsilon t} \quad (\varepsilon \neq 0, |\varepsilon| \leq 1).$$

We assume  $\varepsilon_1 \neq 1$  and  $\varepsilon_k \neq 0$ , which ensures the convergence of the integral.

For positive integers  $k_1, \dots, k_n$  and  $a_1, \dots, a_n \in R_m$ , we see by expanding  $\zeta/(1 - \zeta t)$  into the geometric series and performing the integral repeatedly the identity

$$\begin{aligned} I(\underbrace{0, \dots, 0}_{k_1-1}, \zeta^{a_1}, \underbrace{0, \dots, 0}_{k_2-1}, \zeta^{a_2}, \dots, \underbrace{0, \dots, 0}_{k_n-1}, \zeta^{a_n}) \\ = \sum_{\mu_1=1}^{\infty} \cdots \sum_{\mu_n=1}^{\infty} \frac{\zeta^{a_1 \mu_1} \zeta^{a_2 \mu_2} \cdots \zeta^{a_n \mu_n}}{(\mu_1 + \cdots + \mu_n)^{k_1} (\mu_2 + \cdots + \mu_n)^{k_2} \cdots \mu_n^{k_n}}, \end{aligned}$$

which is nothing but the multiple  $L$ -value  $L_{\text{III}}(k_1, \dots, k_n; a_1, \dots, a_n)$ . Written as an iterated integral, we have

$$\begin{aligned} (5) \quad L_{\text{III}}(k_1, \dots, k_n; a_1, \dots, a_n) &= \underbrace{\int_0^1 \frac{dt}{t} \cdots \int_0^t \frac{dt}{t}}_{k_1-1} \int_0^t \frac{\zeta^{a_1}}{1 - \zeta^{a_1} t} dt \\ &\quad \cdot \int_0^t \frac{dt}{t} \cdots \int_0^t \frac{\zeta^{a_{n-1}}}{1 - \zeta^{a_{n-1}} t} dt \underbrace{\int_0^t \frac{dt}{t} \cdots \int_0^t \frac{dt}{t}}_{k_n-1} \int_0^t \frac{\zeta^{a_n}}{1 - \zeta^{a_n} t} dt. \end{aligned}$$

## 1.2. Algebraic setup.

To formulate the various relations of MLV's, we adopt an algebraic setup developed by Hoffman [H] and used in [IKZ]. Consider the non-commutative polynomial algebra

$$\mathcal{A} := \mathcal{Q}\langle x, y_a; a \in R_m \rangle$$

in  $m+1$  indeterminates  $x, y_a$  ( $a \in R_m$ ). We should remark that it is sometimes necessary to enlarge the field of coefficients to a certain extension of  $\mathcal{Q}$ , depending on the class of functions  $f_i$  involved in the definitions of  $L_{\text{III}}$  or  $L_*$ . For our purpose, however, the field  $\mathcal{Q}$  is sufficient. We also define subalgebras  $\mathcal{A}^1$  and  $\mathcal{A}^0$  of  $\mathcal{A}$  by

$$\mathcal{A}^1 = \mathcal{Q} + \sum_{a \in R_m} \mathcal{A} y_a$$

and

$$\mathcal{A}^0 = \mathcal{Q} + \sum_{a \in R_m} x \mathcal{A} y_a + \sum_{\substack{a, b \in R_m \\ b \neq 0}} y_b \mathcal{A} y_a.$$

For an integer  $k \geq 1$  and  $a \in R_m$ , put  $z_{k,a} = x^{k-1} y_a$ . Then the algebra  $\mathcal{A}^1$  is freely generated by  $z_{k,a}$  for all  $k \geq 1$  and  $a \in R_m$ . We write  $\mathcal{A}_m, \mathcal{A}_m^0$ , and  $\mathcal{A}_m^1$  for  $\mathcal{A}, \mathcal{A}^0$ , and  $\mathcal{A}^1$  respectively, if the index  $m$  should be specified.

Now define “evaluation” maps  $\mathcal{L}_* : \mathcal{A}^0 \rightarrow \mathcal{C}$  and  $\mathcal{L}_{\text{III}} : \mathcal{A}^0 \rightarrow \mathcal{C}$  by

$$\mathcal{L}_*(x^{k_1-1} y_{a_1} x^{k_2-1} y_{a_2} \cdots x^{k_n-1} y_{a_n}) = L_*(k_1, \dots, k_n; a_1, \dots, a_n)$$

and

$$\mathcal{L}_{\text{III}}(x^{k_1-1} y_{a_1} x^{k_2-1} y_{a_2} \cdots x^{k_n-1} y_{a_n}) = L_{\text{III}}(k_1, \dots, k_n; a_1, \dots, a_n),$$

both of which being extended  $\mathcal{Q}$ -linearly. We define the harmonic product  $*$  on  $\mathcal{A}^1$  inductively by

$$1 * w = w * 1 = w,$$

$$z_{k,a}w_1 * z_{l,b}w_2 = z_{k,a}(w_1 * z_{l,b}w_2) + z_{l,b}(z_{k,a}w_1 * w_2) + z_{k+l,a+b}(w_1 * w_2),$$

for all  $k, l \geq 1$ ,  $a, b \in R_m$ , and any words  $w_1, w_2 \in \mathcal{A}^1$ , together with  $\mathbf{Q}$ -bilinearity. In a similar manner as in [H], the space  $\mathcal{A}^1$  equipped with this product is shown to become a commutative algebra and  $\mathcal{A}^0$  a subalgebra. We denote these algebras by  $\mathcal{A}_*^1$  and  $\mathcal{A}_*^0$ . As in the case of multiple zeta values, the multiplication law of the series  $L_*(\mathbf{k}, \mathbf{a})$  is stated as the evaluation map  $\mathcal{L}_*$  on  $\mathcal{A}^0$  is an algebra homomorphism with respect to the harmonic product  $*$ :

$$(6) \quad \mathcal{L}_*(w_1 * w_2) = \mathcal{L}_*(w_1)\mathcal{L}_*(w_2).$$

For instance, the harmonic product

$$x^{k_1-1}y_{a_1} * x^{k_2-1}y_{a_2} = x^{k_1-1}y_{a_1}x^{k_2-1}y_{a_2} + x^{k_2-1}y_{a_2}x^{k_1-1}y_{a_1} + x^{k_1+k_2-1}y_{a_1+a_2}$$

corresponds to

$$L_*(k_1; a_1)L_*(k_2; a_2) = L_*(k_1, k_2; a_1, a_2) + L_*(k_2, k_1; a_2, a_1) + L_*(k_1 + k_2; a_1 + a_2)$$

for admissible index sets  $(k_1; a_1)$  and  $(k_2; a_2)$ .

The other product corresponding to the multiplication of the series  $L_{\boxplus}(\mathbf{k}, \mathbf{a})$  (via its iterated integral expression) is the shuffle product, defined on all of  $\mathcal{A}$  inductively by setting

$$1 \boxplus w = w \boxplus 1 = w,$$

$$uw_1 \boxplus vw_2 = u(w_1 \boxplus vw_2) + v(uw_1 \boxplus w_2),$$

for any words  $w, w_1, w_2 \in \mathcal{A}$  and  $u, v \in \{x, y_a \ (a \in R)\}$ , together with  $\mathbf{Q}$ -bilinearity. This product gives  $\mathcal{A}$  the structure of a commutative  $\mathbf{Q}$ -algebra which we denote by  $\mathcal{A}_{\boxplus}$ . The subspaces  $\mathcal{A}^1$  and  $\mathcal{A}^0$  become subalgebras of  $\mathcal{A}_{\boxplus}$ , denoted by  $\mathcal{A}_{\boxplus}^1$  and  $\mathcal{A}_{\boxplus}^0$  respectively. By the standard shuffle product identity of iterated integrals, the evaluation map  $\mathcal{L}_{\boxplus}$  is an algebra homomorphism:

$$(7) \quad \mathcal{L}_{\boxplus}(w_1 \boxplus w_2) = \mathcal{L}_{\boxplus}(w_1)\mathcal{L}_{\boxplus}(w_2)$$

for all  $w_1, w_2 \in \mathcal{A}^0$ .

As an example of the shuffle product, we give, for any admissible index sets  $(k_1; a_1), (k_2; a_2)$ ,

$$\begin{aligned} x^{k_1-1}y_{a_1} \boxplus x^{k_2-1}y_{a_2} \\ = \sum_{j=0}^{k_2-1} \binom{k_1-1+j}{j} x^{k_1+j-1}y_{a_1}x^{k_2-j-1}y_{a_2} + \sum_{j=0}^{k_1-1} \binom{k_2-1+j}{j} x^{k_2+j-1}y_{a_2}x^{k_1-j-1}y_{a_1} \end{aligned}$$

which corresponds to

$$\begin{aligned} (8) \quad & L_{\boxplus}(k_1; a_1)L_{\boxplus}(k_2; a_2) \\ &= \sum_{j=0}^{k_2-1} \binom{k_1-1+j}{j} L_{\boxplus}(k_1+j; k_2-j; a_1, a_2) \\ &+ \sum_{j=0}^{k_1-1} \binom{k_2-1+j}{j} L_{\boxplus}(k_2+j; k_1-j; a_2, a_1). \end{aligned}$$

## 2. Finite and extended double shuffle relations.

### 2.1. Finite double shuffle relation.

To connect the two algebra homomorphisms (6) and (7), we define a  $\mathcal{Q}$ -linear endomorphism  $\mathcal{I}$  of  $\mathcal{A}^1$ . First we set

$$\mathcal{I}(x^{k_1-1}y_{a_1}x^{k_2-1}y_{a_2}\cdots x^{k_n-1}y_{a_n}) = x^{k_1-1}y_{a_1}x^{k_2-1}y_{a_1+a_2}\cdots x^{k_n-1}y_{a_1+\cdots+a_n}$$

for any index set  $(\mathbf{k}; \mathbf{a}) = (k_1, \dots, k_n; a_1, \dots, a_n)$ , and then extend this to  $\mathcal{A}^1$  by  $\mathcal{Q}$ -linearity. In terms of the map  $\mathcal{I}$ , the relation (4) in Proposition 1.2 is stated as  $\mathcal{L}_* = \mathcal{L}_{\text{III}} \circ \mathcal{I}$ , i.e.,

$$(9) \quad \mathcal{L}_*(w) = \mathcal{L}_{\text{III}}(\mathcal{I}(w)) \quad \text{for all } w \in \mathcal{A}^0.$$

Then the *finite double shuffle relation* for MLV is stated as

PROPOSITION 2.1 (Finite double shuffle relation). *For any  $w_1, w_2 \in \mathcal{A}^0$ , we have*

$$(10) \quad \mathcal{L}_{\text{III}}(\mathcal{I}(w_1)\text{III}\mathcal{I}(w_2) - \mathcal{I}(w_1 * w_2)) = 0.$$

REMARK. When  $m = 1$ , the map  $\mathcal{I}$  is the identity and this relation is nothing but the finite double shuffle relation of the multiple zeta values.

PROOF. By (6), (9) and (7), we have

$$\mathcal{L}_*(w_1 * w_2) = \mathcal{L}_*(w_1)\mathcal{L}_*(w_2) = \mathcal{L}_{\text{III}}(\mathcal{I}(w_1))\mathcal{L}_{\text{III}}(\mathcal{I}(w_2)) = \mathcal{L}_{\text{III}}(\mathcal{I}(w_1)\text{III}\mathcal{I}(w_2)).$$

On the other hand, the left-hand side equals  $\mathcal{L}_{\text{III}}(\mathcal{I}(w_1 * w_2))$  by (9) and hence the proposition holds.  $\square$

### 2.2. Extension of the evaluation maps $\mathcal{L}_*$ and $\mathcal{L}_{\text{III}}$ .

In the next two subsections, we extend the double shuffle relations by taking the divergent series into the picture, namely by regularizing the divergent series. Since the arguments involved are similar to those developed in [IKZ], all the proofs are sketchy except where the map  $\mathcal{I}$  plays a role.

Algebraically, the regularizations are the following extensions of homomorphisms  $\mathcal{L}_{\text{III}}$  and  $\mathcal{L}_*$  to  $\mathcal{A}^1$ . Owing to the isomorphisms of  $\mathcal{Q}$ -algebras  $\mathcal{A}_*^1 \simeq \mathcal{A}_*^0[y_0]$  and  $\mathcal{A}_{\text{III}}^1 \simeq \mathcal{A}_{\text{III}}^0[y_0]$  (the product of  $y_0$  and elements in  $\mathcal{A}^0$  being  $*$  and  $\text{III}$  respectively), the latter of which is standard and the former can be shown in a similar way as in [H], we have, for  $\# = *$  or  $\text{III}$ , the following map  $\hat{\mathcal{L}}_{\#} : \mathcal{A}_{\#}^1 \rightarrow \mathbf{C}[T]$  uniquely characterized by the properties

- (i)  $\hat{\mathcal{L}}_{\#}$  coincides with  $\mathcal{L}_{\#}$  on  $\mathcal{A}^0$ .
- (ii)  $\hat{\mathcal{L}}_{\#}(y_0) = T$ .
- (iii)  $\hat{\mathcal{L}}_{\#}$  is an algebra homomorphism with respect to the product  $\#$ .

EXAMPLES. For  $a \neq 0$ , we have  $y_0 y_a = y_a * y_0 - y_a y_0 - x y_a$  and thus

$$\hat{\mathcal{L}}_*(y_0 y_a) = L_*(1; a)T - L_*(1, 1; a, 0) - L_*(2; a),$$

whereas from  $y_0 y_a = y_a \text{III} y_0 - y_a y_0$  we have

$$\hat{\mathcal{L}}_{\text{III}}(y_0 y_a) = L_{\text{III}}(1; a)T - L_{\text{III}}(1, 1; a, 0).$$

As examples of degree 2, we have

$$\begin{aligned} y_0^2 y_a &= \frac{1}{2} y_a * y_0^{*2} - (xy_a + y_a y_0) * y_0 + \frac{1}{2} x^2 y_a \\ &\quad - \frac{1}{2} xy_0 y_a + xy_a y_0 + \frac{1}{2} y_a x y_0 + y_a y_0^2 \quad (a \neq 0) \end{aligned}$$

and hence

$$\begin{aligned} \hat{\mathcal{L}}_*(y_0^2 y_a) &= \frac{1}{2} L_*(1; a) T^2 - (L_*(2; a) + L_*(1, 1; a, 0)) T + \frac{1}{2} L_*(3; a) \\ &\quad - \frac{1}{2} L_*(2, 1; 0, a) + L_*(2, 1; a, 0) + \frac{1}{2} L_*(1, 2; a, 0) + L_*(1, 1, 1; a, 0, 0). \end{aligned}$$

On the other hand, the equation

$$(11) \quad y_0^2 y_a = \frac{1}{2} y_a \mathbb{I} y_0^2 - y_a y_0 \mathbb{I} y_0 + y_a y_0^2$$

gives

$$\hat{\mathcal{L}}_{\mathbb{I}}(y_0^2 y_a) = \frac{1}{2} L_{\mathbb{I}}(1; a) T^2 - L_{\mathbb{I}}(1, 1; a, 0) T + L_{\mathbb{I}}(1, 1, 1; a, 0, 0).$$

Analytically, these maps have the following interpretations. For  $R > 0$  and an index set  $(\mathbf{k}; \mathbf{a}) = (k_1, \dots, k_n; a_1, \dots, a_n)$ , put

$$L_*^R(k_1, \dots, k_n; a_1, \dots, a_n) = \sum_{R > m_1 > m_2 > \dots > m_n > 0} \frac{\varphi_{a_1}(m_1) \cdots \varphi_{a_n}(m_n)}{m_1^{k_1} m_2^{k_2} \cdots m_n^{k_n}}.$$

If  $(\mathbf{k}, \mathbf{a})$  is admissible, then  $L_*^R(\mathbf{k}, \mathbf{a})$  converges to  $L_*(\mathbf{k}, \mathbf{a})$  as  $R \rightarrow \infty$ . Let  $\mathcal{L}_{\mathbf{k}, \mathbf{a}}^*(T) \in \mathbf{C}[T]$  denote the polynomial  $\hat{\mathcal{L}}_*(w)$  for the word  $w = x^{k_1-1} y_{a_1} \cdots x^{k_n-1} y_{a_n} \in \mathcal{A}^1$  corresponding to the (not necessarily admissible) index set  $(\mathbf{k}, \mathbf{a})$ . Then, in a similar manner as in [IKZ, §2], we see that  $\mathcal{L}_{\mathbf{k}, \mathbf{a}}^*(T)$  is the unique polynomial in  $\mathbf{C}[T]$  such that

$$\lim_{R \rightarrow \infty} R^\delta (L_R^*(\mathbf{k}, \mathbf{a}) - \mathcal{L}_{\mathbf{k}, \mathbf{a}}^*(\log R + \gamma)) = 0$$

for some  $\delta > 0$ . Here  $\gamma$  denotes the Euler constant. We see by induction that, for the index set  $(\mathbf{k}; \mathbf{a}) = (\overbrace{1, \dots, 1}^s, \overbrace{\mathbf{k}'; 0, \dots, 0}^s, \mathbf{a}')$  with an admissible  $(\mathbf{k}'; \mathbf{a}')$ ,

$$\mathcal{L}_{\mathbf{k}, \mathbf{a}}^*(T) = L_*(\mathbf{k}', \mathbf{a}') \frac{T^s}{s!} + (\text{terms of lower degree}).$$

More precisely, we can show also by induction that the coefficient of  $T^i$  is in the  $\mathbf{Q}$ -vector space spanned by the  $L$ -values of weight  $k - i$ ,  $k$  being the weight of  $\mathbf{k}$ .

On the other hand, the polynomial  $\hat{\mathcal{L}}_{\mathbb{I}}(w)$  measures the divergence of the integral (5). More precisely, for an index set  $(\mathbf{k}; \mathbf{a}) = (k_1, \dots, k_n; a_1, \dots, a_n)$ , define a multi-logarithmic function by

$$(12) \quad Li_{\mathbf{k}, \mathbf{a}}(t) = \sum_{m_1 > m_2 > \dots > m_n > 0} \frac{t^{m_1} \varphi_{a_1}(m_1 - m_2) \cdots \varphi_{a_{n-1}}(m_{n-1} - m_n) \varphi_{a_n}(m_n)}{m_1^{k_1} m_2^{k_2} \cdots m_n^{k_n}},$$

which is absolutely convergent for  $|t| < 1$ . This is equal to the integral (5) with the endpoint 1 of the outer integral replaced by  $t$ . Let  $\mathcal{L}_{\mathbf{k}, \mathbf{a}}^{\mathbb{I}}(T) \in \mathbf{C}[T]$  denote the poly-

nomial  $\hat{\mathcal{L}}_{\mathfrak{w}}(w)$  for  $w = x^{k_1-1}y_{a_1} \cdots x^{k_n-1}y_{a_n} \in \mathcal{A}^1$ . Then  $\mathcal{L}_{\mathbf{k}, \mathbf{a}}^{\mathfrak{w}}(T)$  is the unique polynomial satisfying

$$(13) \quad \lim_{t \rightarrow 1-0} (1-t)^{-\delta} (Li_{\mathbf{k}, \mathbf{a}}(t) - \mathcal{L}_{\mathbf{k}, \mathbf{a}}^{\mathfrak{w}}(-\log(1-t))) = 0 \quad \text{for some } \delta > 0.$$

Also, we have

$$\mathcal{L}_{\mathbf{k}, \mathbf{a}}^{\mathfrak{w}}(T) = L_{\mathfrak{w}}(\mathbf{k}', \mathbf{a}') \frac{T^s}{s!} + (\text{terms of lower degree}),$$

where  $\mathbf{k}', \mathbf{a}'$  and  $s$  have the same meaning as above, and the coefficient of  $T^i$  is in the  $\mathbf{Q}$ -vector space spanned by the  $L$ -values of weight  $k-i$ ,  $k$  being the weight of  $\mathbf{k}$ . Proofs of these facts are again similar to the case of multiple zeta values.

The key identity of Zagier in [IKZ], which relates the two types of regularizations, holds true for our setting, if modified by taking the map  $\mathcal{I}$  into account. Define a  $\mathbf{C}$ -linear map  $\rho : \mathbf{C}[T] \rightarrow \mathbf{C}[T]$  by

$$\rho(T^v) = P_v(T) \quad (v = 0, 1, 2, \dots)$$

where

$$P_v(T) = \sum_{j=0}^v \binom{v}{j} \Gamma^{(j)}(1) (T+\gamma)^{v-j},$$

$\Gamma^{(j)}(s)$  being the  $j$ th derivative of the gamma function  $\Gamma(s)$ . By using generating functions, the definition amounts to saying that the image of  $\rho$  of each monomials  $T^v$  is given by (the identity in  $\mathbf{C}[T][[u]]$ )

$$(14) \quad \rho(e^{Tu}) = \sum_{v=0}^{\infty} \frac{\rho(T^v)}{v!} u^v = \Gamma(1+u) e^{(T+\gamma)u}.$$

THEOREM 2.2. On  $\mathcal{A}^1$ , we have

$$(15) \quad \hat{\mathcal{L}}_{\mathfrak{w}} \circ \mathcal{I} = \rho \circ \hat{\mathcal{L}}_*$$

PROOF. For  $\mathbf{a} = (a_1, a_2, \dots, a_n)$ , put  $\tilde{\mathbf{a}} = (a_1, a_2 - a_1, \dots, a_n - a_{n-1})$ . Noting the identities

$$\begin{aligned} Li_{\mathbf{k}, \mathbf{a}}(x) &= \sum_{m=n}^{\infty} \left( \sum_{m > m_2 > \dots > m_n > 0} \frac{\varphi_{a_1}(m-m_2) \cdots \varphi_{a_{n-1}}(m_{n-1}-m_n) \varphi_{a_n}(m_n)}{m^{k_1} m_2^{k_2} \cdots m_n^{k_n}} \right) x^m \\ &= \sum_{m=n}^{\infty} \left( \sum_{m > m_2 > \dots > m_n > 0} \frac{\varphi_{a_1}(m) \varphi_{a_2-a_1}(m_2) \cdots \varphi_{a_n-a_{n-1}}(m_n)}{m^{k_1} m_2^{k_2} \cdots m_n^{k_n}} \right) x^m \\ &= \sum_{m=n}^{\infty} (L_*^{m+1}(\mathbf{k}, \tilde{\mathbf{a}}) - L_*^m(\mathbf{k}, \tilde{\mathbf{a}})) x^m \\ &= \sum_{m=n+1}^{\infty} (x^{m-1} - x^m) L_*^m(\mathbf{k}, \tilde{\mathbf{a}}) \\ &= (x^{-1} - 1) \sum_{m=n+1}^{\infty} L_*^m(\mathbf{k}, \tilde{\mathbf{a}}) x^m, \end{aligned}$$

the argument in [IKZ] works almost literally and we obtain the identity

$$\mathcal{L}_{\mathbf{k}, \mathbf{a}}^{\mathfrak{W}}(T) = \rho(\mathcal{L}_{\mathbf{k}, \mathbf{a}}^*(T)),$$

that is to say, for  $w = x^{k_1-1}y_{a_1} \cdots x^{k_n-1}y_{a_n} \in \mathcal{A}^1$ , we have

$$\hat{\mathcal{L}}_{\mathfrak{W}}(w) = \rho(\hat{\mathcal{L}}_*(x^{k_1-1}y_{a_1}x^{k_2-1}y_{a_2-a_1} \cdots x^{k_n-1}y_{a_n-a_{n-1}})) = \rho(\hat{\mathcal{L}}_*(\mathcal{J}^{-1}(w))).$$

Replacing  $w$  by  $\mathcal{J}(w)$ , we obtain the desired identity.  $\square$

Note that the identity (15) restricts to (9) on  $\mathcal{A}^0$ .

### 2.3. Regularized double shuffle relation.

With the help of Theorem 2.2 we can generalize the double shuffle relation (Proposition 2.1). The case for  $m = 1$  has been treated in [IKZ]. Let  $\text{reg}_{\mathfrak{W}}^T : \mathcal{A}_{\mathfrak{W}}^1 \rightarrow \mathcal{A}_{\mathfrak{W}}^0[T]$  be the  $\mathcal{Q}$ -algebra isomorphism which is the composition of the isomorphisms  $\mathcal{A}_{\mathfrak{W}}^1 \simeq \mathcal{A}_{\mathfrak{W}}^0[y_0] \simeq \mathcal{A}_{\mathfrak{W}}^0[T]$  which sends  $y_0$  to  $T$  and is identity on  $\mathcal{A}_{\mathfrak{W}}^0$ . Note that the map  $\hat{\mathcal{L}}_{\mathfrak{W}}$  defined in the previous section is the composition of  $\text{reg}_{\mathfrak{W}}^T$  and  $\mathcal{L}_{\mathfrak{W}}$  (applied coefficient-wise);  $\hat{\mathcal{L}}_{\mathfrak{W}} = \mathcal{L}_{\mathfrak{W}} \circ \text{reg}_{\mathfrak{W}}^T$ . In other words, an element  $w \in \mathcal{A}_{\mathfrak{W}}^1$  is written uniquely in the form

$$w = w_0 + w_1 \mathfrak{W} y_0 + w_2 \mathfrak{W} y_0^{\mathfrak{W}2} + \cdots + w_n \mathfrak{W} y_0^{\mathfrak{W}n} \quad (w_i \in \mathcal{A}_{\mathfrak{W}}^0)$$

and then

$$\text{reg}_{\mathfrak{W}}^T(w) = w_0 + w_1 T + w_2 T^2 + \cdots + w_n T^n$$

and

$$\hat{\mathcal{L}}_{\mathfrak{W}}(w) = \mathcal{L}_{\mathfrak{W}}(w_0) + \mathcal{L}_{\mathfrak{W}}(w_1)T + \mathcal{L}_{\mathfrak{W}}(w_2)T^2 + \cdots + \mathcal{L}_{\mathfrak{W}}(w_n)T^n.$$

Moreover we define  $\text{reg}_{\mathfrak{W}}(w)$  to be the constant term of  $\text{reg}_{\mathfrak{W}}^T(w)$ ;  $\text{reg}_{\mathfrak{W}}(w) = w_0$  in the above notation. For example, from equation (11) we have  $\text{reg}_{\mathfrak{W}}(y_0^2 y_a) = y_a y_0^2$  ( $a \neq 0$ ). The composition  $\mathcal{L}_{\mathfrak{W}} \circ \text{reg}_{\mathfrak{W}}$  is nothing but to take the constant term of  $\hat{\mathcal{L}}_{\mathfrak{W}}(w)$ .

**THEOREM 2.3** (Regularized double shuffle relations). *For any  $w_0 \in \mathcal{A}^0$  and  $w_1 \in \mathcal{A}^1$ , we have*

$$\mathcal{L}_{\mathfrak{W}}(\text{reg}_{\mathfrak{W}}(\mathcal{J}(w_0) \mathfrak{W} \mathcal{J}(w_1) - \mathcal{J}(w_0 * w_1))) = 0.$$

When  $w_1 \in \mathcal{A}^0$ , this becomes (10).

**PROOF.** By Theorem 2.2 we have

$$\hat{\mathcal{L}}_{\mathfrak{W}}(\mathcal{J}(w_1)) = \rho(\hat{\mathcal{L}}_*(w_1)).$$

Multiplying  $\mathcal{L}_{\mathfrak{W}}(\mathcal{J}(w_0)) = \mathcal{L}_*(w_0) \in \mathcal{C}$  ((9)) on both sides and using the  $\mathcal{C}$ -linearity of  $\rho$ , we have

$$\begin{aligned} \mathcal{L}_{\mathfrak{W}}(\mathcal{J}(w_0))\hat{\mathcal{L}}_{\mathfrak{W}}(\mathcal{J}(w_1)) &= \mathcal{L}_*(w_0)\rho(\hat{\mathcal{L}}_*(w_1)) = \rho(\mathcal{L}_*(w_0)\hat{\mathcal{L}}_*(w_1)) \\ &= \rho(\hat{\mathcal{L}}_*(w_0 * w_1)) = \hat{\mathcal{L}}_{\mathfrak{W}}(\mathcal{J}(w_0 * w_1)). \end{aligned}$$

The left-hand side equals  $\hat{\mathcal{L}}_{\mathfrak{W}}(\mathcal{J}(w_0) \mathfrak{W} \mathcal{J}(w_1))$  and hence we obtain

$$(16) \quad \hat{\mathcal{L}}_{\mathfrak{m}}(\mathcal{I}(w_0) \mathfrak{M} \mathcal{I}(w_1) - \mathcal{I}(w_0 * w_1)) = 0.$$

By taking the constant term, we have

$$\mathcal{L}_{\mathfrak{m}}(\text{reg}_{\mathfrak{m}}(\mathcal{I}(w_0) \mathfrak{M} \mathcal{I}(w_1) - \mathcal{I}(w_0 * w_1))) = 0. \quad \square$$

Substituting  $w_1 = y_0^r$  and using  $\text{reg}_{\mathfrak{m}}(y_0^r) = 0$  (since  $y_0^r = y_0^{\mathfrak{M}r}/r!$ ) in the theorem, we obtain the following apparently weaker relations of MLV's. Rather surprisingly however, these relations imply Theorem 2.2 and hence Theorem 2.3. Also, the relation (16) deduced in the above proof is a consequence of these (and vice versa).

**THEOREM 2.4.** *For all  $r \geq 1$  and  $w_0 \in \mathcal{A}^0$ , we have*

$$(17) \quad \mathcal{L}_{\mathfrak{m}}(\text{reg}_{\mathfrak{m}}(\mathcal{I}(y_0^r * w_0))) = 0.$$

Moreover, we may deduce Theorem 2.2 from these relations. In other words, each of Theorem 2.2, Theorem 2.3, and the current theorem give (together with Proposition 2.1) the same set of linear relations of MLV's.

**PROOF.** The identity is readily shown by specializing  $w_1 = y_0^r$  in Theorem 2.3, as indicated above. The proof of the latter half is carried out in the next section after giving some algebraic preparations necessary.

**EXAMPLE.** Let  $r = 2$  and  $w_0 = y_a$  ( $a \neq 0$ ) in the theorem. We compute the harmonic product as

$$y_0^2 * y_a = xy_a y_0 + y_0 x y_a + y_0^2 y_a + y_0 y_a y_0 + y_a y_0^2$$

and so

$$\mathcal{I}(y_0^2 * y_a) = xy_a^2 + y_0 x y_a + y_0^2 y_a + y_0 y_a^2 + y_a^3.$$

By the regularizations

$$\text{reg}_{\mathfrak{m}}(y_0 x y_a) = -x y_0 y_a - x y_a y_0, \quad \text{reg}_{\mathfrak{m}}(y_0^2 y_a) = y_a y_0^2, \quad \text{reg}_{\mathfrak{m}}(y_0 y_a y_0) = -y_a y_0 y_a - y_a^2 y_0,$$

we have

$$\text{reg}_{\mathfrak{m}}(\mathcal{I}(y_0^2 * y_a)) = xy_a^2 - x y_0 y_a - x y_a y_0 + y_a y_0^2 - y_a y_0 y_a - y_a^2 y_0 + y_a^3.$$

Hence, we obtain the relation

$$\begin{aligned} & L_{\mathfrak{m}}(2, 1; a, a) - L_{\mathfrak{m}}(2, 1; 0, a) - L_{\mathfrak{m}}(2, 1; a, 0) \\ &= -L_{\mathfrak{m}}(1, 1, 1; a, a, a) + L_{\mathfrak{m}}(1, 1, 1; a, a, 0) + L_{\mathfrak{m}}(1, 1, 1; a, 0, a) - L_{\mathfrak{m}}(1, 1, 1; a, 0, 0). \end{aligned}$$

#### 2.4. Proof of Theorem 2.4.

We extend to our  $\mathcal{A}$  or  $\mathcal{A}^1$  various derivations and automorphisms used in [IKZ], which played a vital role in the proof of the extended (regularized) double shuffle relations. Again, we omit the details when the argument is identical to the one given in [IKZ].

Recall that we have set

$$z_{k,a} = x^{k-1} y_a \in \mathcal{A}^1$$

for any positive integer  $k$  and  $a \in R_m$ . Consider the space  $\mathfrak{Z}$  which is the  $\mathcal{Q}$ -linear span of the  $z_{k,a}$  in  $\mathcal{A}$  with  $k \geq 1$ ,  $a \in R_m$ . For each  $b \in R_m$  let  $I_b$  denote the  $\mathcal{Q}$ -linear map of  $\mathfrak{Z}$  defined by

$$I_b(z_{k,a}) = z_{k,a+b} \quad (k \geq 1, a \in R).$$

For  $z \in \mathfrak{Z}$  the map  $\delta_z : \mathcal{A}^1 \rightarrow \mathcal{A}^1$  is defined by

$$\delta_z(w) := z * w - zw \quad (z \in \mathfrak{Z}, w \in \mathcal{A}^1).$$

We observe that  $\delta_z$  is a derivation which commutes with one another, and moreover that  $\delta_z$  extends to a derivation of the non-commutative algebra  $\mathcal{A}$  whose action on generators is given by

$$\delta_z(x) = 0, \quad \delta_z(y_a) = xI_a(z) + y_az \quad (a \in R_m).$$

It is convenient to define a multiplication  $\circ$  on  $\mathfrak{Z}$  with which the space  $\mathfrak{Z}$  becomes a commutative and associative algebra:

$$z \circ z' := z * z' - zz' - z'z \quad (z, z' \in \mathfrak{Z}).$$

For instance, we simply have  $z_{k_1, a_1} \circ z_{k_2, a_2} = z_{k_1+k_2, a_1+a_2}$ .

For  $z \in \mathfrak{Z}$ , define  $\Phi_z : \widehat{\mathcal{A}^1} \rightarrow \widehat{\mathcal{A}^1}$  by

$$\Phi_z(w) := (1 - z) \left( \frac{1}{1 - z} * w \right) \quad (z \in \mathfrak{Z}, w \in \widehat{\mathcal{A}^1}).$$

Here,  $\widehat{\mathcal{A}^1}$  is the completion of  $\mathcal{A}^1$ , i.e., the closure of  $\mathcal{A}^1$  in the non-commutative power series ring  $\widehat{\mathcal{A}}$ , and we denote the element  $1 + z + z^2 + z^3 + \cdots$  in  $\widehat{\mathcal{A}^1}$  by  $1/(1 - z)$ . The map  $\Phi_z$  is an automorphism of  $\widehat{\mathcal{A}^1}$  as non-commutative algebra and is related to the derivation  $\delta$  above by the identity

$$(18) \quad \Phi_z(w) = \exp(\delta_t)(w),$$

where

$$t = \log_{\circ}(1 + z) := \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} (\underbrace{z \circ \cdots \circ z}_n).$$

Note that, because the  $\delta_t$  is a derivation of  $\widehat{\mathcal{A}}$  which raises degree, its exponential

$$\exp(\delta_t) = \sum_{n=0}^{\infty} \frac{\delta_t^n}{n!}$$

is an automorphism of non-commutative algebra  $\widehat{\mathcal{A}}$ , as is seen from the Leibniz rule. The identity (18) then shows that the  $\Phi_z$  extends to an automorphism of non-commutative algebra  $\widehat{\mathcal{A}}$ . We know from [IKZ] that

$$\Phi_z(x) = x, \quad \Phi_z(x + y_0) = (x + y_0)(1 - z)^{-1}.$$

We shall compute  $\Phi_z(x + y_a)$  ( $a \in R_m$ ) in the following.

LEMMA 2.5. For  $z \in \mathfrak{Z}$  and  $a \in R_m$ , we have

$$\begin{aligned}\Phi_z(x + y_a) &= y_a(1 - z)^{-1} + x(1 + I_a(z)(1 - z)^{-1}) \\ &= y_a(1 - z)^{-1} + x + (z \circ y_a)(1 - z)^{-1}.\end{aligned}$$

PROOF. Set  $t = \log_{\circ}(1 + z)$ . Since  $t * y_a = ty_a + y_at + t \circ y_a$ , we have

$$\delta_t(y_a) = t * y_a - ty_a = y_at + t \circ y_a.$$

We can easily prove by induction on  $n$  that

$$(19) \quad \delta_t^n(y_a) = y_at^{*n} + w_n$$

with

$$(20) \quad w_n = \sum_{r=1}^n \binom{n}{r} (\overbrace{t \circ \cdots \circ t}^r \circ y_a) t^{*(n-r)}.$$

We have, by (18) and (19),

$$\begin{aligned}\Phi_z(x + y_a) &= \sum_{n=0}^{\infty} \frac{1}{n!} \delta_t^n(x + y_a) = x + y_a + \sum_{n=1}^{\infty} \frac{1}{n!} (y_at^{*n} + w_n) \\ &= y_a \exp_* t + x + \sum_{n=1}^{\infty} \frac{1}{n!} w_n,\end{aligned}$$

and by (20)

$$\begin{aligned}\sum_{n=1}^{\infty} \frac{1}{n!} w_n &= \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{r=1}^n \binom{n}{r} (\overbrace{t \circ \cdots \circ t}^r \circ y_a) t^{*(n-r)} \\ &= \sum_{r=1}^{\infty} \sum_{n=r}^{\infty} \frac{t^{\circ r} \circ y_a}{r!} \frac{t^{*(n-r)}}{(n-r)!} \\ &= \{(\exp_{\circ} t - 1) \circ y_a\} \sum_{m=0}^{\infty} \frac{t^{*m}}{m!} \\ &= (z \circ y_a) \exp_* t.\end{aligned}$$

Since  $\exp_* t = (1 - z)^{-1}$  and  $z \circ y_a = xI_a(z)$ , we have the assertion.  $\square$

Next define the map  $d_{\mathfrak{W}} : \mathcal{A} \rightarrow \mathcal{A}$  by putting

$$d_{\mathfrak{W}}(w) = y_0 \mathfrak{W} w - y_0 w \quad (w \in \mathcal{A}).$$

This is a derivation on  $\mathcal{A}$  and its exponential is given by (an identity in  $\mathcal{A}[[u]]$ )

$$(21) \quad \exp(d_{\mathfrak{W}} u)(w) = (1 - y_0 u) \left( \frac{1}{1 - y_0 u} \mathfrak{W} w \right) \quad (w \in \mathcal{A}).$$

Also the  $d_{\mathfrak{m}}$  is related to the regularization map  $\hat{\mathcal{L}}_{\mathfrak{m}}$  by (Proposition 8 in [IKZ])

$$(22) \quad \hat{\mathcal{L}}_{\mathfrak{m}}\left(\frac{1}{1-y_0u}w_0\right) = \mathcal{L}_{\mathfrak{m}}(\exp(-d_{\mathfrak{m}})(w_0))e^{Tu},$$

where  $w_0 \in \mathcal{A}^0$  and the identity is in  $\mathbf{C}[T][[u]]$ , the map  $\hat{\mathcal{L}}$  being extended coefficient-wise.

We now give a proof of Theorem 2.4. Set

$$(23) \quad \Delta_u = \exp(-d_{\mathfrak{m}}) \circ \mathcal{J} \circ \Phi_{y_0u},$$

where  $u$  is a formal parameter (the symbol  $\circ$  here denotes the composition of  $\mathbf{Q}$ -linear mappings). We should stress that, unlike the case of multiple zeta values, the map  $\Delta_u$  is *not* an algebra homomorphism because of the insertion of  $\mathcal{J}$ , but only a  $\mathbf{Q}$ -linear map. Replacing  $w$  with  $\Delta_u(w)$  in (21), we have

$$\mathcal{J} \circ \Phi_{y_0u}(w) = (1-y_0u) \left( \frac{1}{1-y_0u} \mathfrak{m} \Delta_u(w) \right).$$

Here the left-hand side equals

$$\mathcal{J} \left( (1-y_0u) \left( \frac{1}{1-y_0u} * w \right) \right) = (1-y_0u) \mathcal{J} \left( \frac{1}{1-y_0u} * w \right).$$

Therefore

$$(24) \quad \mathcal{J} \left( \frac{1}{1-y_0u} * w \right) = \frac{1}{1-y_0u} \mathfrak{m} \Delta_u(w).$$

Note that, since the map  $\Phi_{y_0u}$  preserves  $\mathcal{A}^0$  and  $\mathcal{J}(y_0^m w) = y_0^m \mathcal{J}(w)$  for any  $w \in \mathcal{A}$ , we have  $\Delta_u(w_0) \in \mathcal{A}^0$  if  $w_0 \in \mathcal{A}^0$ . Setting  $w = w_0 \in \mathcal{A}^0$  in (24) and taking  $\text{reg}_{\mathfrak{m}}$  of both hand sides, we have

$$(25) \quad \text{reg}_{\mathfrak{m}} \left( \mathcal{J} \left( \frac{1}{1-y_0u} * w_0 \right) \right) = \Delta_u(w_0).$$

Replacing  $w_0$  with  $\mathcal{J}(\Phi_{y_0u}(w_0))$  in (22), we get

$$\begin{aligned} \text{reg}_{\mathfrak{m}}^T \left( \mathcal{J} \left( \frac{1}{1-y_0u} \Phi_{y_0u}(w_0) \right) \right) &= \text{reg}_{\mathfrak{m}}^T \left( \frac{1}{1-y_0u} \mathcal{J}(\Phi_{y_0u}(w_0)) \right) \\ &= \exp(-d_{\mathfrak{m}}u)(\mathcal{J}(\Phi_{y_0u}(w_0)))e^{Tu} \\ &= \Delta_u(w_0)e^{Tu}. \end{aligned}$$

This yields

$$(26) \quad \hat{\mathcal{L}}_{\mathfrak{m}} \circ \mathcal{J} \left( \frac{1}{1-y_0u} \Phi_{y_0u}(w_0) \right) = \mathcal{L}_{\mathfrak{m}}(\Delta_u(w_0))e^{Tu}.$$

On the other hand, we have the identity (the equation (5.7) in [IKZ])

$$(27) \quad (\rho \circ \hat{\mathcal{L}}_*) \left( \frac{1}{1 - y_0 u} \Phi_{y_0 u}(w_0) \right) = e^{Tu} \mathcal{L}_*(w_0).$$

Therefore by using (26), (27) and (25),

$$\begin{aligned} & (\hat{\mathcal{L}}_{\mathfrak{m}} \circ \mathcal{J} - \rho \circ \hat{\mathcal{L}}_*) \left( \frac{1}{1 - y_0 u} \Phi_{y_0 u}(w_0) \right) = (\mathcal{L}_{\mathfrak{m}}(\Delta_u(w_0)) - \mathcal{L}_*(w_0)) e^{Tu} \\ &= \left\{ \mathcal{L}_{\mathfrak{m}} \left( \text{reg}_{\mathfrak{m}} \left( \mathcal{J} \left( \frac{1}{1 - y_0 u} * w_0 \right) \right) \right) - \mathcal{L}_*(w_0) \right\} e^{Tu} \\ &= \left\{ \mathcal{L}_{\mathfrak{m}} \left( \text{reg}_{\mathfrak{m}} \left( \mathcal{J} \left( \sum_{r=0}^{\infty} u^r (y_0^r * w_0) \right) \right) \right) - \mathcal{L}_*(w_0) \right\} e^{Tu} \\ &= \left\{ \mathcal{L}_{\mathfrak{m}} \left( \text{reg}_{\mathfrak{m}} \left( \mathcal{J} \left( \sum_{r=1}^{\infty} (y_0^r * w_0) u^r \right) \right) \right) + \mathcal{L}_{\mathfrak{m}}(\text{reg}_{\mathfrak{m}}(\mathcal{J}(w_0))) - \mathcal{L}_*(w_0) \right\} e^{Tu} \\ &= \sum_{r=1}^{\infty} \mathcal{L}_{\mathfrak{m}}(\text{reg}_{\mathfrak{m}}(\mathcal{J}(y_0^r * w_0))) u^r e^{Tu} + (\mathcal{L}_{\mathfrak{m}} \circ \mathcal{J}(w_0) - \mathcal{L}_*(w_0)) e^{Tu}. \end{aligned}$$

Note that we have derived this identity in purely algebraic way. Therefore, since the last term on the right vanishes by (9) and since  $y_0^r \Phi_{y_0}(w_0)$  ( $r \geq 0$ ) generate  $\mathcal{A}^1$  if  $w_0$  runs through  $\mathcal{A}^0$ , the relations (15) and (17) are equivalent. This proves Theorem 2.4.  $\square$

Applying (9) to the second formula in the last equalities, we obtain the following corollary which we will need later.

**COROLLARY 2.6.** *For  $w_0 \in \mathcal{A}^0$  we have*

$$\mathcal{L}_{\mathfrak{m}}((\Delta_u - \mathcal{J})(w_0)) = 0.$$

### 3. Derivation relations.

In this section  $z$  denotes  $x + y_0$ ;  $z = x + y_0$ . For an element  $f \in X\mathcal{Q}[[X]]$ , let  $\partial_f$  be the derivation on  $\mathcal{A}$  defined by

$$\begin{cases} \partial_f(x) = x \frac{f(z)}{z} y_0, \\ \partial_f(y_a) = -x \frac{f(z)}{z} y_a + y_a \frac{f(z)}{z} y_0 - y_a \frac{f(z)}{z} y_a \quad (a \in R_m). \end{cases}$$

We often use the formula

$$\partial_f(x + y_a) = (x + y_a) \frac{f(z)}{z} (y_0 - y_a).$$

Let  $\partial_n$  ( $n = 1, 2, \dots$ ) be the particular derivation corresponding to  $f = X^n$ :  $\partial_n = \partial_{X^n}$ . The action on the algebra generators is given by

$$\begin{cases} \partial_n(x) = x(x + y_0)^{n-1}y_0, \\ \partial_n(y_a) = -x(x + y_0)^{n-1}y_a + y_a(x + y_0)^{n-1}y_0 - y_a(x + y_0)^{n-1}y_a \quad (a \in R_m). \end{cases}$$

Now we state the derivation relations of MLV's\*.

**THEOREM 3.1.** *For any  $w_0 \in \mathcal{A}^0$  and  $n \geq 1$ , we have*

$$\mathcal{L}_{\mathfrak{m}}(\partial_n(w_0)) = 0.$$

**EXAMPLE.** Before proving the theorem, we give some examples. Let  $a \neq 0$  (in  $R$ ). By

$$\partial_1(y_a^2) = -xy_a^2 - y_axy_a + y_ay_0y_a + y_a^2y_0 - 2y_a^3$$

and

$$\partial_2(y_a) = -x^2y_a - xy_0y_a + y_axy_0 - y_axy_a + y_ay_0y_0 - y_ay_0y_a,$$

we have

$$\begin{aligned} L_{\mathfrak{m}}(2, 1; a, a) + L_{\mathfrak{m}}(1, 2; a, a) \\ = L_{\mathfrak{m}}(1, 1, 1; a, 0, a) + L_{\mathfrak{m}}(1, 1, 1; a, a, 0) - 2L_{\mathfrak{m}}(1, 1, 1; a, a, a) \end{aligned}$$

and

$$\begin{aligned} L_{\mathfrak{m}}(3; a) + L_{\mathfrak{m}}(2, 1; 0, a) + L_{\mathfrak{m}}(1, 2; a, a) + L_{\mathfrak{m}}(1, 1, 1; a, 0, a) \\ = L_{\mathfrak{m}}(1, 2; a, 0) + L_{\mathfrak{m}}(1, 1, 1; a, 0, 0) \end{aligned}$$

respectively.

To prove the theorem, we introduce the corresponding automorphisms. For  $h \in 1 + X\mathcal{Q}[[X]]$ , let  $\hat{A}_h$  denote the automorphism of the non-commutative completed  $\mathcal{Q}$ -algebra  $\hat{\mathcal{A}}$  defined by

$$\begin{aligned} \hat{A}_h(x) &= x \left( 1 + \frac{h(z) - 1}{z} y_0 \right)^{-1}, \\ \hat{A}_h(x + y_a) &= (x + y_a) \left( 1 + \frac{h(z) - 1}{z} (y_0 - y_a) \right)^{-1}. \end{aligned}$$

As in [IKZ, §7], the derivation  $\partial_f$  and the automorphism  $\hat{A}_h$  are related by

$$\hat{A}_h = \exp(-\partial_f) \quad \text{with } f = \log(h).$$

Consider the specific automorphism  $\hat{A}_{1+uX}$  ( $u$  being a parameter). By the identity  $\log(1 + uX) = \sum_{n=1}^{\infty} (-1)^{n-1} u^n X^n / n$ , the automorphism  $\hat{A}_{1+uX}$  and the derivations  $\{\partial_n\}$  are related by

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\*The case  $n = 1$  and a part of  $n = 2$  were established by T. Koura [Ko].

$$(28) \quad \hat{\Delta}_{1+uX} = \exp\left(-\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} u^n \partial_n\right).$$

The key identity that enables us to connect the double shuffle story in the last section to the derivations  $\partial_n$  is the following. Recall the definition (23) of  $\Delta_u$ .

PROPOSITION 3.2. *For any  $w \in \mathcal{A}$ , we have*

$$\Delta_u(w) = \hat{\Delta}_{1+uX}(\mathcal{J}(w)).$$

Here, the map  $\mathcal{J}$  is extended to  $\mathcal{A}$  by

$$\mathcal{J}(x^{k_1-1}y_{a_1}x^{k_2-1}y_{a_2}\cdots x^{k_n-1}y_{a_n}x^l) = x^{k_1-1}y_{a_1}x^{k_2-1}y_{a_1+a_2}\cdots x^{k_n-1}y_{a_1+\cdots+a_n}x^l.$$

PROOF. As remarked before, this is not an identity of homomorphisms and so we have to check the images of general monomials in  $\mathcal{A}$  on both sides coincide. The identity for  $w = x$  holds true since we have  $\Delta_u(x) = x(1 + uy_0)^{-1}$  as in [IKZ]. Let  $a \in R_m$ . Lemma 2.5 implies

$$(29) \quad \Phi_{uy_0}(x + y_a) = y_a(1 - uy_0)^{-1} + x(1 + uy_a(1 - uy_0)^{-1}).$$

Then,

$$\begin{aligned} \mathcal{J}(\Phi_{uy_0}(x + y_a)) &= y_a(1 - uy_a)^{-1} + x(1 + uy_a(1 - uy_a)^{-1}) \\ &= (x + y_a)(1 - uy_a)^{-1}. \end{aligned}$$

By the definition of  $\Delta_u$ , we find

$$\Delta_u(x + y_a) = \exp(-d_{\mathbb{W}}u)((x + y_a)(1 - uy_a)^{-1}).$$

It is easily shown from the identities  $d_{\mathbb{W}}^n x = n!xy_0^n$  and  $d_{\mathbb{W}}^n y_a = n!y_a y_0^n$  that

$$\exp(-d_{\mathbb{W}}u)(x) = x(1 + uy_0)^{-1}, \quad \exp(-d_{\mathbb{W}}u)(y_a) = y_a(1 + uy_0)^{-1}.$$

Since  $\exp(-d_{\mathbb{W}}u)$  is an automorphism of the non-commutative algebra  $\hat{\mathcal{A}}$ , we have

$$\begin{aligned} \Delta_u(x + y_a) &= (x + y_a)(1 + uy_0)^{-1}(1 - uy_a(1 + uy_0)^{-1})^{-1} \\ &= (x + y_a)(1 + u(y_0 - y_a))^{-1}. \end{aligned}$$

Here the last expression coincides with  $\hat{\Delta}_{1+uX}(x + y_a)$ . Therefore we have

$$\Delta_u(w) = \hat{\Delta}_{1+uX}(\mathcal{J}(w))$$

for  $w = x, y_a$ .

Let  $w = x^{k_1-1}y_{a_1}\cdots x^{k_n-1}y_{a_n}x^{l-1}$  be a monomial in  $\mathcal{A}$  with  $k_1, \dots, k_n, l$  positive integers and  $a_1, \dots, a_n \in R_m$ . Then, taking the identities

$$\Phi_{uy_0}(y_a) = (1 + ux)y_a(1 - uy_0)^{-1} \quad (a \in R_m) \text{ and } \Phi_{uy_0}(x) = x$$

into account, we have

$$\Phi_{uy_0}(w) = x^{k_1-1}\Phi_{uy_0}(y_{a_1})x^{k_2-1}\cdots x^{k_n-1}\Phi_{uy_0}(y_{a_n})x^{l-1}.$$

For simplicity write  $Y_a = (1 + ux)y_a(1 - uy_a)^{-1}$  for  $a \in R_m$ . Using this notation, we have

$$\mathcal{J}(\Phi_{uy_0}(w)) = x^{k_1-1} Y_{a_1} x^{k_2-1} Y_{a_1+a_2} \cdots x^{k_n-1} Y_{a_1+\cdots+a_n} x^{l-1}.$$

Since

$$\exp(-d_{\mathfrak{m}}u)(Y_a) = \Delta_u(y_a) = \hat{\Delta}_{1+uX}(y_a) \quad (a \in R_m),$$

$$\begin{aligned} \Delta_u(w) &= \exp(-d_{\mathfrak{m}}u)(\mathcal{J}(\Phi_{uy_0}(w))) \\ &= \exp(-d_{\mathfrak{m}}u)(x^{k_1-1}) \exp(-d_{\mathfrak{m}}u)(Y_{a_1}) \cdots \\ &\quad \exp(-d_{\mathfrak{m}}u)(x^{k_n-1}) \exp(-d_{\mathfrak{m}}u)(Y_{a_1+\cdots+a_n}) \exp(-d_{\mathfrak{m}}u)(x^{l-1}) \\ &= \hat{\Delta}_{1+uX}(x^{k_1-1}) \hat{\Delta}_{1+uX}(y_{a_1}) \cdots \hat{\Delta}_{1+uX}(y_{a_1+\cdots+a_n}) \hat{\Delta}_{1+uX}(x^{l-1}) \\ &= \hat{\Delta}_{1+uX}(x^{k_1-1} y_{a_1} x^{k_2-1} y_{a_1+a_2} \cdots x^{k_n-1} y_{a_1+\cdots+a_n} x^{l-1}) \\ &= \hat{\Delta}_{1+uX}(\mathcal{J}(w)). \end{aligned}$$

□

PROOF OF THEOREM 3.1. By Proposition 3.2 and (28), we have

$$\Delta_u = (\hat{\Delta}_{1+uX} \circ \mathcal{J}) = \exp\left(-\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} u^n \partial_n\right) \circ \mathcal{J}$$

and hence

$$\begin{aligned} -\sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} u^n \partial_n &= \log(\Delta_u \circ \mathcal{J}^{-1}) = \log(1 + \Delta_u \circ \mathcal{J}^{-1} - 1) \\ &= \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} (\Delta_u \circ \mathcal{J}^{-1} - 1)^n. \end{aligned}$$

Corollary 2.6 gives

$$\mathcal{L}_{\mathfrak{m}}((\Delta_u \circ \mathcal{J}^{-1} - 1)^n(w_0)) = 0$$

for all  $n \geq 1$  and  $w_0 \in \mathcal{A}^0$  and therefore we conclude

$$\mathcal{L}_{\mathfrak{m}}(\partial_n(w_0)) = 0.$$

□

REMARK. In [G2, Proposition 2.13] Goncharov gives the “distribution relations”, which reads for  $l|m$  and  $a_i \in lR_m$

$$\begin{aligned} L_{\mathfrak{m}}(k_1, k_2, \dots, k_n; a_1, a_2, \dots, a_n) \\ = l^{k_1+k_2+\cdots+k_n-n} \sum_{b_i \in R_m, lb_i=a_i} L_{\mathfrak{m}}(k_1, k_2, \dots, k_n; b_1, b_2, \dots, b_n) \end{aligned}$$

(when each  $L$ -value converges). The authors do not know whether there is some exact relationship between these and the relations discussed in our paper or not.

## 4. Applications.

### 4.1. Principal part of multiple $L$ -functions.

For any index set  $(\mathbf{k}; \mathbf{a}) = (k_1, \dots, k_n; a_1, \dots, a_n)$  not necessarily admissible, we define “multiple  $L$ -functions”  $L_{\mathbf{k}, \mathbf{a}}^*(s)$  and  $L_{\mathbf{k}, \mathbf{a}}^{\square}(s)$  of single complex variable  $s$  by the Dirichlet series

$$L_{\mathbf{k}, \mathbf{a}}^*(s) = \sum_{m_1 > m_2 > \dots > m_n > 0} \frac{\varphi_{a_1}(m_1) \varphi_{a_2}(m_2) \cdots \varphi_{a_n}(m_n)}{m_1^{k_1+s} m_2^{k_2} \cdots m_n^{k_n}}$$

and

$$L_{\mathbf{k}, \mathbf{a}}^{\square}(s) = \sum_{m_1 > m_2 > \dots > m_n > 0} \frac{\varphi_{a_1}(m_1 - m_2) \cdots \varphi_{a_{n-1}}(m_{n-1} - m_n) \varphi_{a_n}(m_n)}{m_1^{k_1+s} m_2^{k_2} \cdots m_n^{k_n}}.$$

The series are absolutely convergent for  $\operatorname{Re}(s) > 0$  and can be extended to a meromorphic function of  $s$  in a similar fashion as in [AK]. If the index  $(\mathbf{k}; \mathbf{a})$  is admissible, then both functions are holomorphic at  $s = 0$  having the values

$$L_{\mathbf{k}, \mathbf{a}}^*(0) = L_*(\mathbf{k}; \mathbf{a}) \quad \text{and} \quad L_{\mathbf{k}, \mathbf{a}}^{\square}(0) = L_{\square}(\mathbf{k}; \mathbf{a}),$$

while for non-admissible index they have a pole at  $s = 0$ . As a matter of fact, the two functions are essentially the same and related with each other by

$$(30) \quad L_{\mathbf{k}, \mathbf{a}}^{\square}(s) = L_{\mathbf{k}, I^{-1}(\mathbf{a})}^*(s),$$

where  $I$  is the bijection on the set  $R_m^n$  defined by  $I(a_1, a_2, \dots, a_n) = (a_1, a_1 + a_2, \dots, a_1 + a_2 + \dots + a_n)$ . If  $\mathbf{a} = (\underbrace{0, 0, \dots, 0}_n)$ , then both  $L_{\mathbf{k}, \mathbf{a}}^*(s)$  and  $L_{\mathbf{k}, \mathbf{a}}^{\square}(s)$  give the same function which is denoted by  $\zeta(k_1 + s, k_2, \dots, k_n)$ .

In the following, we show that the principal parts at  $s = 0$  of  $L_{\mathbf{k}, \mathbf{a}}^*(s)$  and of  $\Gamma(s+1)L_{\mathbf{k}, \mathbf{a}}^{\square}(s)$  are completely determined by the polynomials  $\mathcal{L}_{\mathbf{k}, \mathbf{a}}^*(T)$  and  $\mathcal{L}_{\mathbf{k}, \mathbf{a}}^{\square}(T)$  defined in §2.2. (Recall the descriptions of the coefficients of these polynomials given there.)

**THEOREM 4.1.** (i) Write the polynomial  $\mathcal{L}_{\mathbf{k}, \mathbf{a}}^*(T)$  as

$$\mathcal{L}_{\mathbf{k}, \mathbf{a}}^*(T) = \sum_{j=0}^v \frac{b_j}{j!} (T - \gamma)^j,$$

where  $\gamma$  is the Euler constant. Then the principal part of  $L_{\mathbf{k}, \mathbf{a}}^*(s)$  at  $s = 0$  is given by

$$L_{\mathbf{k}, \mathbf{a}}^*(s) = \sum_{j=0}^v \frac{b_j}{s^j} + O(s) \quad (s \rightarrow 0).$$

(ii) Write the polynomial  $\mathcal{L}_{\mathbf{k}, \mathbf{a}}^{\square}(T)$  as

$$\mathcal{L}_{\mathbf{k}, \mathbf{a}}^{\square}(T) = \sum_{j=0}^v \frac{c_j}{j!} T^j.$$

Then the principal part of  $\Gamma(s+1)L_{\mathbf{k},\mathbf{a}}^{\text{III}}(s)$  at  $s=0$  is given by

$$\Gamma(s+1)L_{\mathbf{k},\mathbf{a}}^{\text{III}}(s) = \sum_{j=0}^v \frac{c_j}{s^j} + O(s) \quad (s \rightarrow 0).$$

REMARK. As for the precise order of pole at  $s=0$ , we only know it is at most  $t$ , where  $t$  is the number given by  $(\mathbf{k}; \mathbf{a}) = (\overbrace{1, \dots, 1}^t, \mathbf{k}'; \overbrace{0, \dots, 0}^t, \mathbf{a}')$  with an admissible  $(\mathbf{k}'; \mathbf{a}')$ . When  $L_*(\mathbf{k}', \mathbf{a}') \neq 0$  (resp.  $L_{\text{III}}(\mathbf{k}', \mathbf{a}') \neq 0$ ), the order of pole at  $s=0$  of  $L_{\mathbf{k},\mathbf{a}}^*(s)$  (resp.  $L_{\mathbf{k},\mathbf{a}}^{\text{III}}(s)$ ) is exactly  $t$ . If  $\mathbf{a}' = (0, 0, \dots, 0)$ , this is the case, but in general, we do not know when the  $L$ -values vanish.

PROOF. We first establish the assertion (ii). When  $\mathbf{k} = (\underbrace{1, 1, \dots, 1}_n)$  and  $\mathbf{a} = (\underbrace{0, 0, \dots, 0}_n)$ , the polynomial  $\mathcal{L}_{\mathbf{k},\mathbf{a}}^{\text{III}}(T)$  is equal to  $T^n/n!$  (since  $y_0^n = y_0^{\text{III}}/n!$ ) and thus the formula becomes

$$(31) \quad \Gamma(s+1)\zeta(s+1, \underbrace{1, \dots, 1}_{n-1}) = \frac{1}{s^n} + O(s) \quad (s \rightarrow 0),$$

which was proved in [AK, Proposition 4 (ii)]. The general case is obtained from this as follows.

From the definition of the function  $Li_{\mathbf{k},\mathbf{a}}(t)$  given in §2.2, it is immediate to see that

$$(32) \quad \Gamma(s)L_{\mathbf{k},\mathbf{a}}(s) = \int_0^\infty t^{s-1} Li_{\mathbf{k},\mathbf{a}}(e^{-t}) dt.$$

As stated in (13), we have the estimate

$$|Li_{\mathbf{k},\mathbf{a}}(e^{-t}) - \mathcal{L}_{\mathbf{k},\mathbf{a}}^{\text{III}}(-\log(1 - e^{-t}))| < C(1 - e^{-t})^\delta$$

as  $t \rightarrow +0$  with some constants  $C, \delta > 0$ . With this, we may conclude that the principal part of  $\Gamma(s+1)L_{\mathbf{k},\mathbf{a}}(s) = s\Gamma(s)L_{\mathbf{k},\mathbf{a}}(s)$  at  $s=0$  coincides with that of

$$s \int_0^\infty t^{s-1} \mathcal{L}_{\mathbf{k},\mathbf{a}}^{\text{III}}(-\log(1 - e^{-t})) dt = s \sum_{j=0}^v \frac{c_j}{j!} \int_0^\infty t^{s-1} (-\log(1 - e^{-t}))^j dt.$$

Since  $(-\log(1 - e^{-t}))^j/j! = Li_{\underbrace{1, \dots, 1}_j}(e^{-t})$  (cf. [AK, Lemma 1 (ii)]), we have by (32) and (31),

$$s \int_0^\infty t^{s-1} \frac{(-\log(1 - e^{-t}))^j}{j!} dt = \Gamma(s+1)\zeta(s+1, \underbrace{1, \dots, 1}_{j-1}) = \frac{1}{s^j} + O(s) \quad (\text{as } s \rightarrow 0).$$

We therefore have

$$s \int_0^\infty t^{s-1} \mathcal{L}_{\mathbf{k},\mathbf{a}}^{\text{III}}(-\log(1 - e^{-t})) dt = \sum_{j=0}^v \frac{c_j}{s^j} + O(s) \quad (\text{as } s \rightarrow 0)$$

and the assertion (ii) is proved.

For (ii), we note the relation which follows from (30):

$$L_{\mathbf{k}, \mathbf{a}}^*(s) = L_{\mathbf{k}, I(\mathbf{a})}^{\text{III}}(s) = \frac{1}{\Gamma(s+1)} \Gamma(s+1) L_{\mathbf{k}, I(\mathbf{a})}^{\text{III}}(s).$$

By (i), the principal part of  $\Gamma(s+1) L_{\mathbf{k}, I(\mathbf{a})}^{\text{III}}(s)$  corresponds to  $\mathcal{L}_{\mathbf{k}, I(\mathbf{a})}^{\text{III}}(T)$ , which is equal to  $(\hat{\mathcal{L}}_{\text{III}} \circ \mathcal{J})(w)$  with  $w$  = the word corresponding to  $(\mathbf{k}; \mathbf{a})$  in the previous notation. By Theorem 2.2, this in turn equals  $(\rho \circ \hat{\mathcal{L}}_*)(w)$ . Recalling the definition (14) of  $\rho$ , we see by a routine computation which we omit that this gives the assertion (i).  $\square$

REMARK. Tracing the above calculations carefully, we may deduce Theorem 2.2 from equation (31).

#### 4.2. Some examples of relations among multiple $L$ -values.

We restrict ourselves to the cases  $m = 3$  and 4 and give results having a flavor of “sum formula”. Let  $\chi_3$  and  $\chi_4$  be the unique non-trivial Dirichlet characters mod 3 and mod 4 respectively. The following result was first proved by M. Nishi [N] by a method of manipulating the defining series.

PROPOSITION 4.2 (Nishi). *For any integer  $n \geq 2$ , we have*

$$\begin{aligned} & \sum_{i=1}^{n-1} (2^i + 2) L_{\text{III}}(i, n-i; \chi_3, \chi_3) + 2 L_{\text{III}}(1, n-1; \chi_3, \chi_3) + 2 L_{\text{III}}(n-1, 1; \chi_3, \chi_3) \\ &= (n-1) L_{\text{III}}(n; \chi_3^2) \quad (= (n-1)(1-3^{-n})\zeta(n)) \end{aligned}$$

and

$$\begin{aligned} & \sum_{i=1}^{n-1} 2^i L_{\text{III}}(i, n-i; \chi_4, \chi_4) + 2 L_{\text{III}}(1, n-1; \chi_4, \chi_4) \\ &= (n-1) L_{\text{III}}(n; \chi_4^2) \quad (= (n-1)(1-2^{-n})\zeta(n)). \end{aligned}$$

PROOF. We give a proof of the second identity, the first being obtained similarly. First we note that from the shuffle product identity similar to (8), we have

$$\begin{aligned} & L_{\text{III}}(i; f_1) L_{\text{III}}(n-i; f_2) \\ &= \sum_{j=i}^{n-1} \binom{j-1}{j-i} L_{\text{III}}(j; n-j; f_1, f_2) + \sum_{j=n-i}^{n-1} \binom{j-1}{j-n+i} L_{\text{III}}(j; n-j; f_2, f_1) \end{aligned}$$

and by summing up

$$\sum_{i=1}^{n-1} L_{\text{III}}(i; f_1) L_{\text{III}}(n-i; f_2) = \sum_{i=1}^{n-1} 2^{i-1} (L_{\text{III}}(i, n-i; f_1, f_2) + L_{\text{III}}(i, n-i; f_2, f_1))$$

for any  $f_1, f_2$  with  $\hat{f}_1(0) = \hat{f}_2(0) = 0$ . By this we find

$$(33) \quad \sum_{i=1}^{n-1} 2^i L_{\text{III}}(i, n-i; \chi_4, \chi_4) = \sum_{i=1}^{n-1} L_{\text{III}}(i; \chi_4) L_{\text{III}}(n-i; \chi_4).$$

The product on the right is rewritten by the harmonic product as

$$(34) \quad \begin{aligned} L_{\mathfrak{W}}(i; \chi_4) L_{\mathfrak{W}}(n-i; \chi_4) &= L_*(i; \chi_4) L_*(n-i; \chi_4) \\ &= 2L_*(i, n-i; \chi_4, \chi_4) + L_*(n; \chi_4^2). \end{aligned}$$

Hence the left-hand side of the equation to be proved is equal to

$$2 \left( \sum_{i=1}^{n-1} L_*(i, n-i; \chi_4, \chi_4) + L_{\mathfrak{W}}(1, n-1; \chi_4, \chi_4) \right) + (n-1)L_*(n; \chi_4^2),$$

so we have to show

$$\sum_{i=1}^{n-1} L_*(i, n-i; \chi_4, \chi_4) + L_{\mathfrak{W}}(1, n-1; \chi_4, \chi_4) = 0.$$

Now since  $\hat{\chi}_4(1) = 1$ ,  $\hat{\chi}_4(3) = -1$  ( $\hat{\chi}_4(0) = \hat{\chi}_4(2) = 0$ ), Proposition 1.2 gives

$$(35) \quad \begin{aligned} L_*(i, n-i; \chi_4, \chi_4) &= -\frac{1}{4} (L_{\mathfrak{W}}(i, n-i; \varphi_1, \varphi_2) - L_{\mathfrak{W}}(i, n-i; \varphi_1, \varphi_0) \\ &\quad - L_{\mathfrak{W}}(i, n-i; \varphi_3, \varphi_0) + L_{\mathfrak{W}}(i, n-i; \varphi_3, \varphi_2)). \end{aligned}$$

Specializing  $k_1 = 1$ ,  $k_2 = n-1$  in (8) and using

$$\begin{aligned} L_{\mathfrak{W}}(1; \varphi_{a_1}) L_{\mathfrak{W}}(n-1; \varphi_{a_2}) &= L_*(1; \varphi_{a_1}) L_*(n-1; \varphi_{a_2}) \\ &= L_*(1, n-1; \varphi_{a_1}, \varphi_{a_2}) + L_*(n-1, 1; \varphi_{a_2}, \varphi_{a_1}) + L_*(n; \varphi_{a_1+a_2}) \\ &= L_{\mathfrak{W}}(1, n-1; \varphi_{a_1}, \varphi_{a_2}) + L_{\mathfrak{W}}(n-1, 1; \varphi_{a_2}, \varphi_{a_1}) + L_{\mathfrak{W}}(n; \varphi_{a_1+a_2}), \end{aligned}$$

we have

$$(36) \quad \begin{aligned} \sum_{i=1}^{n-1} L_{\mathfrak{W}}(i, n-i; \varphi_{a_1}, \varphi_{a_2}) \\ &= L_{\mathfrak{W}}(1, n-1; \varphi_{a_1}, \varphi_{a_1+a_2}) + L_{\mathfrak{W}}(n-1, 1; \varphi_{a_2}, \varphi_{a_1+a_2}) \\ &\quad + L_{\mathfrak{W}}(n; \varphi_{a_1+a_2}) - L_{\mathfrak{W}}(n-1, 1; \varphi_{a_2}, \varphi_{a_1}). \end{aligned}$$

Suppose  $n > 2$ . Then we may put  $a_2 = 0$  in (36) and from equations (33), (34), (35), and (36) we obtain

$$\begin{aligned} \sum_{i=1}^{n-1} L_*(i, n-i; \chi_4, \chi_4) &= -\frac{1}{4} (L_{\mathfrak{W}}(1, n-1; \varphi_1, \varphi_3) - L_{\mathfrak{W}}(1, n-1; \varphi_1, \varphi_1) \\ &\quad - L_{\mathfrak{W}}(1, n-1; \varphi_3, \varphi_3) + L_{\mathfrak{W}}(1, n-1; \varphi_3, \varphi_1)) \\ &= -L_{\mathfrak{W}}(1, n-1; \chi_4, \chi_4). \end{aligned}$$

This gives the desired equation. For  $n = 2$ , what we have to show is the equation

$$4L_{\mathfrak{W}}(1, 1; \chi_4, \chi_4) = L_{\mathfrak{W}}(2; \chi_4^2).$$

Since

$$\begin{aligned} L_{\mathfrak{m}}(2; \chi_4^2) &= L_*(2; \chi_4^2) = L_*(1; \chi_4)^2 - 2L_*(1, 1; \chi_4, \chi_4) \\ &= L_{\mathfrak{m}}(1; \chi_4)^2 - 2L_*(1, 1; \chi_4, \chi_4) = 2L_{\mathfrak{m}}(1, 1; \chi_4, \chi_4) - 2L_*(1, 1; \chi_4, \chi_4), \end{aligned}$$

we need to show  $L_*(1, 1; \chi_4, \chi_4) = -L_{\mathfrak{m}}(1, 1; \chi_4, \chi_4)$ . Now by (35), we have

$$(37) \quad \begin{aligned} L_*(1, 1; \chi_4, \chi_4) &= -\frac{1}{4}(L_{\mathfrak{m}}(1, 1; \varphi_1, \varphi_2) - L_{\mathfrak{m}}(1, 1; \varphi_1, \varphi_0) \\ &\quad - L_{\mathfrak{m}}(1, 1; \varphi_3, \varphi_0) + L_{\mathfrak{m}}(1, 1; \varphi_3, \varphi_2)). \end{aligned}$$

Applying Theorem 3.1 for  $n = 1$ ,  $w_0 = y_a$  ( $a \neq 0$ ), we get

$$L_{\mathfrak{m}}(1, 1; \varphi_a, \varphi_0) = L_{\mathfrak{m}}(1, 1; \varphi_a, \varphi_a) + L_{\mathfrak{m}}(2; \varphi_a).$$

Using this and (36), we see the right-hand side of (37) is equal to

$$\begin{aligned} &-\frac{1}{4}(-L_{\mathfrak{m}}(1, 1; \varphi_1, \varphi_1) - L_{\mathfrak{m}}(1, 1; \varphi_3, \varphi_3) + L_{\mathfrak{m}}(1, 1; \varphi_1, \varphi_3) + L_{\mathfrak{m}}(1, 1; \varphi_3, \varphi_1)) \\ &= -L_*(1, 1; \chi_4, \chi_4). \end{aligned} \quad \square$$

We have found numerically the following rather curious identities. (The first was found by Nishi [N].) In particular, the sums on the left are suggested to belong to the ring generated by the Riemann zeta values.

Set  $\zeta_2(s) = (1 - 2^{-s})\zeta(s)$  and  $\zeta_3(s) = (1 - 3^{-s})\zeta(s)$ . For odd  $n$ , we conjecturally have

$$\begin{aligned} \sum_{i=2}^{n-2} L_{\mathfrak{m}}(i, n-i; \chi_3, \chi_3) &\stackrel{?}{=} -\frac{n-3}{2}\zeta_3(n) + \sum_{m=1}^{(n-3)/2} \frac{3^{2m}-3}{3^{2m}-1}\zeta_3(2m)\zeta_3(n-2m), \\ \sum_{i=1}^{n-1} L_{\mathfrak{m}}(i, n-i; \chi_4, \chi_4) &\stackrel{?}{=} \frac{1}{2}\zeta_2(n) + \sum_{m=1}^{(n-3)/2} \frac{1-2^{1-2m}}{2^{2m}-1}\zeta_2(2m)\zeta_2(n-2m). \end{aligned}$$

As for a general “sum formula”, only we could show is the following relation, which can be deduced by applying shuffle product identity on the right-hand side. For any  $f$  with  $\hat{f}(0) = 0$ , we abbreviate  $L_{\mathfrak{m}}(k_1, k_2, \dots, k_n; f, f, \dots, f)$  as  $L_{\mathfrak{m}}(k_1, k_2, \dots, k_n; f)$ .

**PROPOSITION 4.3.** *Let  $k, n$  be positive integers with  $1 \leq n \leq k$ . Then we have*

$$\sum_{k_1+\dots+k_n=k} L_{\mathfrak{m}}(k_1, \dots, k_n; f) = \sum_{j=0}^{n-1} \frac{(-1)^{n+j-1}}{j!} L_{\mathfrak{m}}(1, f)^j L_{\mathfrak{m}}(\underbrace{1, \dots, 1}_{n-1-j}, k+1-n; f),$$

where the summation on the left is taken over all positive integers  $k_1, \dots, k_n$  with  $k_1 + \dots + k_n = k$ .

#### 4.3. A connection to the Drinfeld associator.

As is fairly known, the regularized multiple zeta values are closely related to the so-called Drinfeld KZ associator. We recall briefly the definition of the Drinfeld KZ

associator [D]. For more detail, see *e.g.*, [Ka, Chapter XIX]. Consider the linear differential equation

$$(38) \quad G'(t) = \left( \frac{X}{t} + \frac{Y}{1-t} \right) G(t)$$

and its unique solutions  $G_0(t)$  and  $G_1(t)$  such that

$$G_0(t) \sim t^X \quad (t \rightarrow 0) \quad \text{and} \quad G_1(t) \sim (1-t)^{-Y} \quad (t \rightarrow 1).$$

The Drinfeld KZ associator  $\Phi_{KZ}(X, Y)$  is an element in  $R\langle\langle X, Y \rangle\rangle$  defined by

$$\Phi_{KZ}(X, Y) = G_1(t)^{-1} G_0(t).$$

The alleged relation to MZV's is then stated as follows: The coefficient of each word  $W$  in  $\Phi_{KZ}(X, Y)$  is equal to the regularized zeta value of  $w$ . Here  $w$  is the word obtained from  $W$  by replacing  $X$  with  $x$  and  $Y$  with  $y$ . Here, the regularization means to take the constant term of  $w$ , viewed as an element in the shuffle algebra  $\mathcal{Q}\langle x, y \rangle_{\text{III}}$  which is isomorphic to the polynomial algebra  $\mathfrak{h}_{\text{III}}^0[x, y]$  over  $\mathfrak{h}_{\text{III}}^0 = \mathcal{Q} + x\mathcal{Q}\langle x, y \rangle y$ , and then take the corresponding multiple zeta value of this constant term  $\in \mathfrak{h}_{\text{III}}^0$  (see [IKZ] for algebraic computations of the regularizations).

Now consider the following generalization of (38):

$$(39) \quad H'(t) = \frac{X}{t} H(t) + \sum_{a \in R_m} \frac{\zeta^a Y_a}{1 - \zeta^a t} H(t).$$

By using the function  $Li_{k,a}(t)$  defined in (12), we can construct a solution  $H_0(t)$  to (39) such that  $H_0(t) \sim t^X \quad (t \rightarrow 0)$  as follows<sup>†</sup>.

Let  $w \in \mathcal{A}^1$  be the word which corresponds to the index  $(k, a)$  and write  $Li_{k,a}(t)$  as  $Li_w(t)$ . Recall the map  $w \mapsto Li_w(t)$  is a  $\text{III}$ -homomorphism from  $\mathcal{A}_{\text{III}}^1$  to the algebra of analytic functions near  $t = 0$ . We extend this homomorphism (uniquely) to the whole  $\mathcal{A}_{\text{III}}$  by setting  $Li_x(t) = \log(t)$ . Then the series

$$H_0(t) = \sum_{w \in \mathcal{A}} Li_w(t) W,$$

where  $W$  is the capitalized word corresponding to  $w$ , is a solution of (39). We may write out more explicitly the coefficient  $Li_w(t)$  when  $w \notin \mathcal{A}^1$  as in the explicit regularization formula in [IKZ, Corollary to Proposition 10], but we omit it here.

The following question arises naturally and would be very interesting.

**PROBLEM.** Is there an analogous theory of the Drinfeld associator for this differential equation which is closely connected to the regularized multiple  $L$ -values?<sup>‡</sup>

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<sup>†</sup>We have made an erroneous statement on the solution in [AK2]. The authors would very much like to thank Hidekazu Furusho and Jun-ichi Okuda, who independently pointed out the error and supplied the correct form of the solution.

<sup>‡</sup>Recently Okuda announced such a theory exists at least for small  $m$ . See his forthcoming article for the details.

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