

# Introduction to Multiple Zeta Values, I

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► What is the arithmetic nature of a real number  $x \in \mathbb{R}$ ? We can ask whether  $x$  is rational, or algebraic, or transcendental. Very little is known in terms of decimal expansions.

There is a recent conjecture of Kontsevich and Zagier in their joint paper “periods” (*Mathematics Unlimited - 2001 and Beyond*. Engquist, B.; Schmid, W., (Eds.), Springer (2000), 771–808). But it is too vague to be disproved by counterexamples.

**Examples.**  $x = \sum_{n \geq 0} \frac{P(n)}{Q(n)}$ , where  $P, Q \in \mathbb{Z}[x]$ , with  $\deg Q \geq \deg P + 2$ . We omit those finitely many  $n \geq 0$  with  $Q(n) = 0$  in the sum.

*Example 1.*  $\sum_{n \geq 1} \frac{1}{n(n+1)}$ . This is a telescoping series, where the general term can be written as  $n^{-1} - (n+1)^{-1}$ . So the sum converges to 1, a rational number.

Similarly, we can consider  $\sum \frac{1}{(n+a)(n+b)}$ , with  $a, b \in \mathbb{Z}$ ,  $a \neq b$ .

*Example 2.*  $\sum_{n \geq 0} \frac{1}{(2n+1)(2n+2)}$ . The general term is  $(2n+1)^{-1} - (2n+2)^{-1}$ . The series is now seen to be convergent to  $\log 2$ , which is transcendental by Hermite-Lindeman.

*Example 3.*  $\sum_{n=0}^{\infty} \frac{1}{(n+1)(2n+1)(4n+1)} = \frac{\pi}{3}$ .

*Example 4.*  $\sum_{n=0}^{\infty} \prod_{i=1}^6 \frac{1}{6n+i} = \frac{1}{4320}(192 \log 2 - 81 \log 3 - 7\pi\sqrt{3})$ .

Write  $\pi$  as  $i \log(-1)$ , we can use Baker’s theorem to see that this number is transcendental. Baker’s theorem asserts that a finite sum  $\sum \beta_i \log \alpha_i$ , with algebraic  $\alpha_i, \beta_i$ , is transcendental whenever the sum is non-zero.

► The work of Adhikari, Saradha, Shorey, Tijdeman.

Consider  $x = \sum_{n \geq 0} \frac{P(n)}{Q(n)}$ , where  $Q$  has only simple rational zeros and  $\deg Q \geq 2 + \deg P$ . Then we can rewrite the series in the following form

$$x = \frac{a}{b} + \sum_{n \geq 0} \sum_{j=1}^m \frac{c_j}{k_j n + r_j},$$

with  $0 < r_j \leq k_j$ .

Define

$$f(z) = \sum_{n \geq 0} \frac{z^n}{kn + r}$$

This can be analyzed by considering  $g(z) = z^r f(z^k)$ , then  $zg'(z) = z^r/(1 - z^k)$ . We then get

$$x = \frac{a}{b} + \sum_{j=1}^m \sum_{l=0}^{k_j-1} \frac{c_j}{k_j} (1 - \zeta_{k_j}^{rj^l}) \log(1 - \zeta_{k_j}^l),$$

where  $\zeta_{k_j} = e(1/k_j)$ ,  $e(z) = \exp(2\pi iz)$ . Thus we conclude that  $x$  is either rational or transcendental. It can never be an algebraic irrationality. The proof also gives a way to decide whether  $x$  is rational or transcendental. If it is rational, it is just  $a/b$ .

*Example.*  $\sum \frac{1}{(5n+1)(5n+3)(5n+5)}$  is transcendental.

*Example.*  $\sum \left( \frac{1}{4n+1} - \frac{3}{4n+2} + \frac{1}{4n+3} + \frac{1}{4n+4} \right)$ . This turns out to be rational as the “transcendental part” is  $\log 2 - \log(1+i) - \log(1-i)$  is 0, but this is not apparent without going through the computations.

► Now consider the case that  $Q$  has distinct roots, but not rational.

*Example.*  $\sum_{n \geq 0} \frac{1}{n^2+1} = \frac{1}{2} + \frac{\pi}{2} \cdot \frac{e^\pi + e^{-\pi}}{e^\pi - e^{-\pi}}$ . This is transcendental by a theorem of Nesterenko:  $\pi$  and  $e^\pi$  are algebraic independent.

**Schanuel’s conjecture.** Let  $x_1, \dots, x_n$  be complex numbers linearly independent over  $\mathbb{Q}$ . Then the transcendence degree of  $\mathbb{Q}(x_1, \dots, x_n, e^{x_1}, \dots, e^{x_n})/\mathbb{Q}$  is at least  $n$ .

*Question.* What is a function field version of this conjecture related to Drinfeld modules?

**Bundschuh’s formula.** For  $s \in \mathbb{Z}$ ,  $s \geq 2$ ,

$$\sum_{|n| \geq 2, n \in \mathbb{Z}} \frac{1}{n^s - 1} = 2 - \frac{\delta_s}{2s} - \frac{\pi i}{s} \sum_{\sigma} \zeta_{\sigma} \frac{e(\zeta_{\sigma}^s) + 1}{e(\zeta_{\sigma}^s) - 1}.$$

Here,  $\delta_s = 1$  or  $2$  depending on  $s$  is odd or even, and  $\zeta_{\sigma} = e(1/s)$ , and  $1 \leq \sigma \leq s$ ,  $\sigma \neq s/2$ .

*Example.* Let  $s = 2$ , then we get  $2 \sum_{n \geq 2} \frac{1}{n^2 - 1} = \frac{3}{2}$  (telescoping).

*Exercise.* Let  $s = 4$ . We get  $2 \sum_{n \geq 2} \frac{1}{n^4 - 1} = \frac{7}{4} - \frac{\pi}{2} \cdot \frac{e^\pi + e^{-\pi}}{e^\pi - e^{-\pi}}$ .

*Proof of Bundschuh’s formula.* We use residue calculus. Consider

$$\frac{1}{2\pi i} \int_{\Gamma_N} \frac{\pi \cot(\pi z)}{z^s - 1} dz = I(N),$$

where  $I_N$  is the square with side length  $2N + 1$  centered at the origin. The poles are  $\mathbb{Z} \cup \mu_s$ . Be careful at  $z = \pm 1$ , where we may have second order poles.

**The case of multiple zeroes for  $Q$ .** For example,

$$\sum_{n \geq 1} \frac{1}{n^2} = \frac{\pi^2}{6}.$$

This can be done by the same method of residue calculus. Here we give a proof of Calabi, which appeared in a recent Bourbaki talk (Cartier, 2001).

Consider

$$\int_0^1 \int_0^1 \frac{dx dy}{1 - x^2 y^2} = \int_0^1 \int_0^1 \sum_{n=0}^{\infty} (x^2 y^2)^n dx dy = \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2}.$$

Now apply change of variables:  $x = \sin u / \cos v$ ,  $y = \sin v / \cos u$ , so that  $dx dy / (1 - x^2 y^2) = du dv$ . The new region of integration is  $0 \leq u \leq \pi/2$ ,  $0 \leq v \leq \pi/2$ ,  $u + v \leq \pi/2$ . This gives that the integral is  $\pi^2/8$ , from where the desired result follows.

**Riemann's zeta.**

$$\zeta(s) = \sum_{n \geq 1} \frac{1}{n^s}.$$

Consider the case that  $s$  is an integer  $\geq 2$ . It was known to Euler that

$$\zeta(2r) = (-1)^{r+1} \frac{2^{2r-1} B_{2r}}{(2r)!} \pi^{2r}$$

for  $r \geq 1$ , where  $\frac{t}{e^t - 1} = \sum_{n=0}^{\infty} \frac{B_n t^n}{n!}$ . In particular,  $B_n \in \mathbb{Q}$ .

From here, we know that  $\zeta(2r)$  are rational multiples of  $\pi^{2r}$ , hence are transcendental. But only relatively recently, it is shown that  $\zeta(3)$  is irrational (Apéry). Now we know that there are infinitely many  $\zeta(2r+1)$ ,  $r \geq 1$  which are irrational (Rivoal, 2000, C.R.A.S.). In fact, the dimension of the  $\mathbb{Q}$ -vector space spanned by  $\zeta(3), \dots, \zeta(a)$ , ( $a$ : odd) is  $\geq \frac{\log a}{1 + \log 2} (1 + o(1))$  (Ball, Rivoal, 2001, Invent. Math.). Moreover, Rivoal and Zudilin showed that one of the 9 numbers  $\zeta(5), \dots, \zeta(21)$  is irrational in June 2001. In July, Zudilin improved 9 to 8, then recently to 4: *one of the 4 numbers  $\zeta(5), \zeta(7), \zeta(9), \zeta(11)$  is irrational.*

**Expectation.** The numbers  $\pi, \zeta(3), \zeta(5), \dots, \zeta(2r+1), \dots$  are algebraically independent.

**Multiple zeta values.** We want to consider

$$\sum_{n_1 > \dots > n_k \geq 1} \frac{1}{n_1^{s_1} \dots n_k^{s_k}} = \zeta(s_1, \dots, s_k) = \zeta(\underline{s}).$$

Here,  $s_1, \dots, s_k \in \mathbb{Z}$ ,  $s_1 \geq 2$ ,  $s_j \geq 1$  for  $2 \leq j \leq k$ . For  $k = 1$ , this reduces to Riemann's zeta function. We call  $k$  the length or depth of  $\underline{s}$ , and  $|\underline{s}| = \sum s_j$  the weight of  $\underline{s}$ .

*Remark.* These multiple zeta values have been considered by J. Écalle in the context of “resurgent series” where he introduced “mould calculus”. Roughly, for each  $\underline{s}$ , he introduced an object  $M^{\underline{s}}$ , in a category, say of modules over a ring  $A$ , with lots of symmetries.

Multiple zeta values have also been considered by N. Nielsen, A.B. Goncharov and D. Zagier.

*Fact.* There are many algebraic relations among  $\zeta(\underline{s})$ .

Now we feel that we have found all the relations and there should be no more. It is not easy to check whether a “new” relation is a consequence of known ones.

*Simple example.* 
$$\zeta(s)\zeta(s') = \sum_{n \geq 1} \frac{1}{n^s} \sum_{m \geq 1} \frac{1}{m^{s'}} = \sum_{n > m} + \sum_{n < m} + \sum_{n=m} = \zeta(s, s') + \zeta(s', s) + \zeta(s + s').$$

This is an example of a quadratic relation, generally of the form

$$\zeta(\underline{s})\zeta(\underline{s}') = \sum_{\underline{\sigma}} \zeta(\underline{\sigma}).$$

Some non-commutative polynomial algebra  $\mathbb{Q}\langle X \rangle$ ,  $X = \{x_0, x_1\}$ , and shuffle products,  $\dots$  will be used to describe the relations.

# Introduction to Multiple Zeta Values, II

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*Remark.* Adhikari-Saradha-Shorey-Tijdeman also considered sums of the form

$$\sum_{n \geq 0} \frac{f(n)}{Q(n)},$$

where  $Q$  is a polynomial with simple rational zeros, and  $f$  is periodic modulo  $q > 0$ , such that the convergence condition is satisfied.

**Corollary.** Let  $\chi$  be a Dirichlet character modulo  $q$ , not principal, then

$$L(\chi, 1) = \sum_{n \geq 1} \frac{\chi(n)}{n}$$

is transcendental.

*Remark.* But this is not a new way to prove the non-vanishing of  $L(\chi, 1)$ .

**Free algebras.**

Let  $K$  be a field (to be specialized to a subfield of  $\mathbb{R}$  later; three main examples:  $\mathbb{Q}$ ,  $\bar{\mathbb{Q}} \cap \mathbb{R}$ ,  $\mathbb{R}$ ).

Let  $X$  be a set. Consider the universal problem of constructing a  $K$ -algebra  $K\langle X \rangle$  and a map  $X \rightarrow K\langle X \rangle$  such that for any  $K$ -algebra  $A$ , any map  $f : X \rightarrow A$ , there is a unique extension  $\bar{f}$  making the diagram

$$\begin{array}{ccc} X & \xrightarrow{f} & A \\ & \searrow & \uparrow \bar{f} \\ & & K\langle X \rangle \end{array}$$

commutative.

If  $X = \{x\}$ , the solution is just that  $K\langle x \rangle = K[x]$ , the polynomial algebra in a single variable. In general polynomial algebras solve the problem if we replace algebras by commutative algebras.

Let  $X^*$  be the set of words on  $X$ , that is, monomials  $x_1 \cdots x_n$ ,  $n \geq 0$ ,  $x_i \in X$ . Denote by  $e$  the empty product. Take  $X^*$  as the basis of  $K\langle X \rangle$  as a  $K$ -vector space. We can think of  $K\langle X \rangle$  as  $K^{(X^*)}$ , the space of functions from  $X^*$  to  $K$  with finite supports.

Thus elements of  $K\langle X \rangle$  are finite sums  $s = \sum_{w \in X^*} (s|w)w$ . The addition is defined componentwise, so  $(s + s'|w) = (s|w) + (s'|w)$ . Multiplication is defined by concatenation, so  $(ss'|w) = \sum_{u,v \in X^*, uv=w} (s|u)(s'|v)$ .

Let  $\mathcal{H} = K\langle X \rangle$ . This is a non-commutative graded algebra. The grading is defined by assigning weight  $n$  to a word  $x_1 \cdots x_n$ . Let  $\mathcal{H}_n$  be the subspace spanned by words of length  $n$ . Clearly,  $\mathcal{H}_n \mathcal{H}_m \subset \mathcal{H}_{n+m}$ .

Most important to us is the case  $X = \{x_0, x_1\}$ . We will write  $\mathcal{H} = K\langle x_0, x_1 \rangle$ .

**Fact.** The algebra  $K\langle Y \rangle$  with  $Y = \{y_1, y_2, \dots\}$  is isomorphic to a subalgebra of  $K\langle x_0, x_1 \rangle$ .

This is very different from the case of free commutative algebras. To see this, we write a map  $Y \rightarrow K\langle X \rangle$  by  $y_s \mapsto x_0^{s-1}x_1$  for  $s \geq 1$ . By the universal property, we get a morphism  $f : K\langle Y \rangle \rightarrow K\langle X \rangle$ . It suffices to show that this is injective, which is not difficult.

The image  $\mathcal{H}^1$  of  $f$  is a subalgebra of  $\mathcal{H}$ , and is precisely the subalgebra spanned by words which end with  $x_1$ . The set of such words is denoted by  $X^*x_1$ . We have  $\mathcal{H}^1 = K.e + \mathcal{H}x_1$ .

*Notation.* For  $\underline{s} = (s_1, \dots, s_k)$ , we write  $y_{\underline{s}} = y_{s_1} \dots y_{s_k}$ .

The words  $y_{s_1} \dots y_{s_k}$  with  $s_1 \geq 2$  are the words which start with  $x_0$  and end with  $x_1$ .

We define the set of *convergent words* to be  $\{e\} \cup (x_0X^*x_1)$ , and a subalgebra  $\mathcal{H}^0 = K.e + x_0\mathcal{H}x_1$ . We have  $\mathcal{H}^0 \subset \mathcal{H}^1 \subset \mathcal{H}$ .

Now assume that  $K \subset \mathbb{R}$ . We define  $\hat{\zeta} : \mathcal{H}^0 \rightarrow \mathbb{R}$  to be the  $K$ -linear map defined by  $\hat{\zeta}(y_{\underline{s}}) = \zeta(\underline{s})$  for  $\underline{s} = (s_1, \dots, s_k)$  with  $s_1 \geq 2$ .

**Goal.** Define a law on  $\mathcal{H}^0$ , denoted by  $*$ , such that

$$\hat{\zeta}(y_{\underline{s}})\hat{\zeta}(y_{\underline{s}'}) = \hat{\zeta}(y_{\underline{s}} * y_{\underline{s}'}).$$

Notice that the left hand side is simply  $\zeta(\underline{s}) \cdot \zeta(\underline{s}')$ .

Now

$$\zeta(\underline{s}) \cdot \zeta(\underline{s}') = \sum_{n_1 > \dots > n_k \geq 1} \frac{1}{n_1^{s_1} \dots n_k^{s_k}} \cdot \sum_{n'_1 > \dots > n'_{k'} \geq 1} \frac{1}{n'_1{}^{s'_1} \dots n'_{k'}{}^{s'_{k'}}}.$$

We rewrite this as  $\sum_{\underline{\sigma}} \zeta(\underline{\sigma})$  and define  $y_{\underline{s}} * y_{\underline{s}'} = \sum_{\underline{\sigma}} y_{\underline{\sigma}}$ .

*Definition.* We define  $*$  by induction on  $k + k'$ : for  $s \geq 2, s' \geq 2$ , and  $u, v \in X^*$ , we define

$$(y_s u) * (y_{s'} v) = y_s(u * (y_{s'} v)) + y_{s'}((y_s u) * v) + y_{s+s'}(u * v).$$

(Cf. the quadratic relation computation for  $\zeta(s)\zeta(s')$ ).

Now we have defined  $*$  on  $\mathcal{H}^0$ . We will extend it to  $\mathcal{H}^1$  and  $\mathcal{H}$ . We do so by defining  $x_0^m * u = u * x_0^m = ux_0^m$ . Then  $\mathcal{H}$  is a commutative algebra for  $(+, *)$ . The commutativity is obvious. This commutative algebra will be denoted by  $\mathcal{H}_*$ , and called the *harmonic algebra*. The subspace  $\mathcal{H}^0$  and  $\mathcal{H}^1$  are subalgebras, denoted by  $\mathcal{H}_*^0$  and  $\mathcal{H}_*^1$ . By definition,  $\hat{\zeta} : \mathcal{H}_*^0 \rightarrow \mathbb{R}$  is a morphism of  $K$ -algebras.

The relation

$$\hat{\zeta}(u * v) = \hat{\zeta}(u) \cdot \hat{\zeta}(v) \quad (\text{stuffle product})$$

is a quadratic relation among zeta values.

*Examples.*

$$\begin{aligned} \zeta(2)^2 &= 2\zeta(2, 2) + \zeta(4), \\ \zeta(2)^3 &= 6\zeta(2, 2, 2) + 3\zeta(2, 4) + 3\zeta(4, 2) + \zeta(6). \end{aligned}$$

**Quasi-symmetric functions.** Consider infinitely many commuting variables  $t_1, \dots, t_n, \dots$  and power series in these variables (with coefficients in  $K$ ). The algebra of such power series is denoted by  $K[[\underline{t}]]$ .

The symmetric functions form a subalgebra  $\text{Sym}$  of  $K[[\underline{t}]]$ , which is spanned by

$$M_{\underline{s}}(\underline{t}) = \sum_{n_1 \geq 1, \dots, n_k \geq 1} t_{n_1}^{s_1} \cdots t_{n_k}^{s_k}.$$

In fact, the  $M_{\underline{s}}$ 's with  $(s_1 \geq \cdots \geq s_k \geq 1)$  form a basis  $\text{Sym}$ .

The algebra  $Q\text{Sym}$  of quasi-symmetric functions is spanned by

$$QM_{\underline{s}}(\underline{t}) = \sum_{n_1 > \cdots > n_k \geq 1} t_{n_1}^{s_1} \cdots t_{n_k}^{s_k},$$

where  $s_1, \dots, s_k \geq 1$ . This contains the symmetric functions as  $M_{\underline{s}} \sim \sum_{\underline{t}} QM_{\underline{t}}$ , where  $\underline{t}$  range over permutations of  $\underline{s}$ .

There is an isomorphism of algebras from  $\mathcal{H}_*^1$  and  $Q\text{Sym}$ , such that  $y_{\underline{s}} \mapsto QM_{\underline{s}}(\underline{t}) = F(y_{\underline{s}})$ , where  $F(y_{\underline{s}}) = \sum_{n_1 > \cdots > n_k \geq 1} t_{n_1}^{s_1} \cdots t_{n_k}^{s_k}$  extended by linearity. We have

$$F(y_{\underline{s}}) \cdot F(y_{\underline{s}'}) = F(y_{\underline{s}} * y_{\underline{s}'}).$$

Hoffman shows that  $\mathcal{H}^*$  is a polynomial algebra on the so-called Lyndon words.

We put an order on  $X^*$  by using the lexicographic order with  $x_0 < x_1$ . For example, for words of length  $\leq 2$ :

$$x_0 < x_0^2 < x_0x_1 < x_1 < x_1x_0 < x_1^2.$$

Then a Lyndon word is a word  $w$  which is smaller than each proper right factor: if  $w = uv$  then  $w < v$ . Lyndon words of length  $\leq 2$  are  $x_0, x_0x_1, x_1$ .

Each Lyndon word different from  $x_0, x_1$  starts with  $x_0$  and ends with  $x_1$ .

*Consequence.* Using this product, we can not get algebraic relations between  $\hat{\zeta}(x_0^2x_1)$  and  $\hat{\zeta}(x_0x_1^2)$  ( $x_0^2x_1$  and  $x_0x_1^2$  are Lyndon words). But the first one is  $\zeta(3)$  and the second one  $\zeta(2, 1)$ , and they are actually the same. Thus we have not captured all relations.

**Exercises.** Check  $\zeta(2, \dots, 2)$  ( $k$  copies of 2's) is equal to  $\frac{\pi^{2k}}{(2k+1)!}$ .

$$\text{Hint. } \sum_{k \geq 0} \frac{\pi^{2k}}{(2k+1)!} z^{2k} (-1)^k = \frac{\sin(\pi z)}{\pi z} = \prod_{n \geq 1} \left(1 - \frac{z^2}{n^2}\right).$$

$$\prod_{n \geq 1} (1 - zt_n) = \sum_{k \geq 0} (-1)^k \lambda_k(\underline{t}) z^k,$$

where  $\lambda_k(\underline{t}) = \sum_{n_1 > \cdots > n_k \geq 1} t_{n_1} \cdots t_{n_k} = QM_{(1, \dots, 1)}$  ( $k$  copies of 1's).

# Introduction to Multiple Zeta Values, III

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► **Chen's iterated integrals.**

Let  $\varphi_1, \dots, \varphi_p$  be holomorphic differential forms on some open set of  $\mathbb{C}$ . We define

$$\int_a^b \varphi_1 \cdots \varphi_p$$

by induction: (when  $p = 1$ , it is the usual integral)

$$\int_a^b \varphi_1 \cdots \varphi_p = \int_a^b \varphi_1(t) \int_a^t \varphi_2 \cdots \varphi_p.$$

By means of a change of variable we may assume that  $a = 0$  and  $b = 1$ .

We have the following explicit formula:

$$\int_0^1 \varphi_1 \cdots \varphi_p = \int_{1 > t_1 > \dots > t_p > 0} \varphi_1(t_1) \cdots \varphi_p(t_p).$$

These iterated integrals occur naturally when one studies product of integrals:

$$\int_0^1 \varphi_1 \int_0^1 \varphi_2 = \int_{1 > t > 0, 1 > u > 0} \varphi_1(t) \varphi_2(u) = \int_{1 > u > t > 0} + \int_{1 > t > u > 0} = \int_0^1 \varphi_1 \varphi_2 + \int_0^1 \varphi_2 \varphi_1.$$

**Lemma.** Define

$$S_{p,q} = \{\sigma \in S_{p+q} : \sigma(1) < \dots < \sigma(p), \sigma(p+1) < \dots < \sigma(p+q)\}.$$

Then

$$\int_0^1 \varphi_1 \cdots \varphi_p \int_0^1 \varphi_{p+1} \cdots \varphi_{p+q} = \sum_{\sigma \in S_{p,q}} \int_0^1 \varphi_{\sigma(1)} \cdots \varphi_{\sigma(p+q)}.$$

The subset  $S_{p,q} \subset S_{p+q}$  is called the set of  $(p, q)$ -shuffles.

**PROOF.** The idea is in the above simple example.

$$\text{LHS} = \int_{1 > t_1 > \dots > t_p > 0, 1 > t_{p+1} > \dots > t_{p+q}} \varphi_1(t_1) \cdots \varphi_{p+q}(t_{p+q}).$$

Now use the fact that the domain of integration is a product of two simplices, and decomposes into the disjoint union of  $\{1 > t_{\sigma(1)} > \dots > t_{\sigma(p+q)}\}$  for  $\sigma \in S_{p,q}$ .

**Lemma.**

$$\int_{x_0}^{x_1} \varphi_1 \cdots \varphi_p = \sum_{j=0}^p \int_x^{x_1} \varphi_1 \cdots \varphi_j \int_{x_0}^x \varphi_{j+1} \cdots \varphi_p.$$

**PROOF.** This is an exercise. Also an exercise: this is not true with  $\int_{x_0}^x \varphi_1 \cdots \varphi_j \int_x^{x_1} \varphi_{j+1} \cdots \varphi_p$ .



► **Polylogarithms.**

The classical polylogarithms are

$$\text{Li}_s(z) = \sum_{n \geq 1} \frac{z^n}{n^s}.$$

Here,  $s \geq 1$  is an integer,  $z \in \mathbb{C}$  is such that  $|z| < 1$  (or  $s \geq 2$  and  $|z| \leq 1$ ). We have  $\zeta(s) = \text{Li}_s(1)$ .

Now

$$\begin{aligned} \text{Li}_1(z) &= \sum_{n \geq 1} \frac{z^n}{n} = -\log(1-z) = \int_0^z \frac{dt}{1-t} \\ z \frac{d}{dz} \text{Li}_s(z) &= \text{Li}_{s-1}(z), \quad s \geq 2. \end{aligned}$$

So

$$\text{Li}_s(z) = \int_0^z \text{Li}_{s-1}(t) \frac{dt}{t}, \quad s \geq 2.$$

By induction,

$$\text{Li}_s(z) = \int_0^z \frac{dt_1}{t_1} \cdots \frac{dt_{s-1}}{t_{s-1}} \frac{dt_s}{1-t_s}.$$

Put  $\omega_0 = dt/t$ ,  $\omega_1 = dt/(1-t)$ , so that

$$\text{Li}_s(z) = \int_0^z \omega_0^{s-1} \omega_1 = \int_0^z \omega_s,$$

where  $\omega_s = \omega_0^{s-1} \omega_1$  for  $s \geq 1$ .

*Multiple polylogarithms in a single variable.* Let  $\underline{s} = (s_1, \dots, s_k)$ . Define

$$\text{Li}_{\underline{s}}(z) = \sum_{n_1 > \dots > n_k \geq 1} \frac{z^{n_1}}{n_1^{s_1} \cdots n_k^{s_k}},$$

where  $s_i \geq 1$  and  $|z| < 1$ . Also we can allow  $|z| \leq 1$  if  $s_1 \geq 2$ . We have  $\text{Li}_{\underline{s}}(1) = \zeta(\underline{s})$ .

Observe

$$\frac{d}{dz} \text{Li}_{\underline{s}}(z) = \frac{1}{z} \text{Li}_{(s_1-1, s_2, \dots, s_k)}(z)$$

if  $s_1 \geq 2$ ;

$$\frac{d}{dz} \text{Li}_{\underline{s}}(z) = \frac{1}{1-z} \text{Li}_{(s_2, \dots, s_k)}(z)$$

if  $s_1 = 1$ . So

$$\text{Li}_{\underline{s}}(z) = \int_0^z \omega_0^{s_1-1} \omega_1 \text{Li}_{(s_2, \dots, s_k)}(t) = \int_0^z \omega_0^{s_1-1} \omega_1 \cdots \omega_0^{s_k-1} \omega_1.$$

For  $\underline{s} = (s_1, \dots, s_k)$ , define  $\omega_{\underline{s}} = \omega_{s_1} \cdots \omega_{s_k}$ , so

$$\text{Li}_{\underline{s}}(z) = \int_0^z \omega_{\underline{s}}.$$

Recall that  $\mathbb{Q} \subset K \subset \mathbb{R}$  and we have defined  $\mathcal{H} = K\langle x_0, x_1 \rangle$ ,  $y_s = x_0^{s-1}x_1$  for  $s \geq 1$ ,  $y_{\underline{s}} = y_{s_1} \cdots y_{s_k}$  for  $\underline{s} = (s_1, \dots, s_k)$ . We have

$$\mathcal{H}^1 = Ke + \mathcal{H}x_1 = \left\{ c_0 + \sum_{\underline{s}} c_{\underline{s}} y_{\underline{s}} : c_0, c_{\underline{s}} \in K \right\}.$$

Now define

$$\widehat{\text{Li}}_{y_{\underline{s}}} = \text{Li}_{\underline{s}}$$

and extend the definition by linearity:

$$\widehat{\text{Li}}_{c_0 + \sum c_{\underline{s}} y_{\underline{s}}} = c_0 + \sum_{\underline{s}} c_{\underline{s}} \text{Li}_{\underline{s}}.$$

Hence  $\widehat{\text{Li}}_u(z)$  is well-defined for  $u \in \mathcal{H}^1$ ,  $|z| < 1$ .

We want to investigate  $\text{Li}_{\underline{s}}(z) \cdot \text{Li}_{\underline{s}'}(z)$ . For  $\underline{s} = (s_1, \dots, s_k)$ , recall  $\omega_{\underline{s}} = \omega_0^{s_1-1} \omega_1 \cdots \omega_0^{s_k-1} \omega_1$ . We can rewrite this as  $\omega_{\epsilon_1} \cdots \omega_{\epsilon_p}$  where  $\epsilon_i \in \{0, 1\}$ , where  $p = \sum s_i$  and  $\#\{i : \epsilon_i = 1\} = k$ .

Recall the lemma:

$$\int_0^z \omega_{\epsilon_1} \cdots \omega_{\epsilon_p} \int_0^z \omega_{\epsilon_{p+1}} \cdots \omega_{\epsilon_{p+q}} = \sum_{\sigma \in S_{p,q}} \int_0^z \omega_{\epsilon_{\sigma(1)}} \cdots \omega_{\epsilon_{\sigma(p+q)}}.$$

Definition of Shuffle  $\text{III}$  on  $\mathcal{H}$  by induction

$$\begin{aligned} e \text{ III } w &= w \text{ III } e = w \\ x_{\epsilon} u \text{ III } x_{\epsilon'} v &= x_{\epsilon} (u \text{ III } x_{\epsilon'} v) + x_{\epsilon'} (x_{\epsilon} u \text{ III } v) \end{aligned}$$

and distributivity. It follows by induction that the shuffle product is commutative. Denote the vector spaces  $\mathcal{H} \supset \mathcal{H}^1 \supset \mathcal{H}^0$  with the shuffle product by

$$\mathcal{H}_{\text{III}} \supset \mathcal{H}_{\text{III}}^1 \supset \mathcal{H}_{\text{III}}^0.$$

**Proposition.** For  $u, v \in \mathcal{H}^1$ ,  $\widehat{\text{Li}}_u(z) \widehat{\text{Li}}_v(z) = \widehat{\text{Li}}_{u \text{ III } v}(z)$ .

**Corollary.** For  $u, v \in \mathcal{H}^0$ ,  $\widehat{\zeta}(u) \widehat{\zeta}(v) = \widehat{\zeta}(u \text{ III } v)$ .

*Examples.*  $\text{Li}_1^n(z) = n! \text{Li}_{\{1\}_n}(z)$ , where  $\{1\}_n = (1, \dots, 1)$  ( $n$  copies).

$$\text{Li}_1(z) \text{Li}_2(z) = 2 \text{Li}_{(2,1)}(z) + \text{Li}_{(1,2)}(z).$$

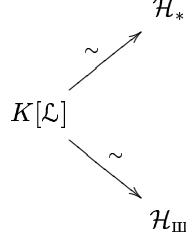
Let  $u = x_1, v = x_0 x_1$ . Then  $u \text{ III } v = 2x_0 x_1^2 + x_1 x_0 x_1$ . This gives the above formula.

$$\text{Li}_2(z)^2 = 4 \text{Li}_{(3,1)}(z) + 2 \text{Li}_{(2,2)}(z).$$

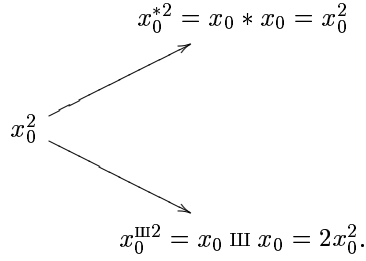
**Collorary.**  $\zeta(2)^2 = 4\zeta(3, 1) + 2\zeta(2, 2)$ . (Shuffle).

Compare with *shuffle*:  $\zeta(2)^2 = 2\zeta(2, 2) + \zeta(4)$ . We get  $\zeta(4) = 4\zeta(3, 1)$ .

The algebra  $\mathcal{H}_{\text{III}}$  was studied by Radford. It is a polynomial algebra with a basis the set of Lyndon words  $\mathcal{L}$ .



Take a simple non-Lyndon word  $x_0^2$ :



*Generating series* for  $\widehat{\text{Li}}_w(z)$ ,  $w \in X^*$ . We need to define  $\widehat{\text{Li}}_w(z)$  for  $w = ux_0^m$ ,  $m \geq 1$ . The trick is

$$\text{“} \int_0^z \frac{dz}{z} \text{”} \mapsto \int_1^z \frac{dz}{z}.$$

So we set

$$\widehat{\text{Li}}_{x_0^m}(z) = \frac{1}{m!} (\log z)^m$$

and define  $\widehat{\text{Li}}_w(z)$  by induction: for  $i = 0, 1$ ,

$$\widehat{\text{Li}}_{x_i u}(z) = \int_0^z \omega_i(t) \text{Li}_u(t).$$

The generating series for  $\widehat{\text{Li}}_w$ :

$$\widehat{\text{Li}}(z) = \sum_{w \in X^*} \widehat{\text{Li}}_w(z) \cdot w$$

is a (non-commutative) power series in  $x_0, x_1$ .

*Differential equation.* On a simply connected open set in  $\mathbb{P}^1$  not containing  $0, 1, \infty$ :

$$\frac{d}{dz} \widehat{\text{Li}}(z) = \left( \frac{x_0}{z} + \frac{x_1}{1-z} \right) \widehat{\text{Li}}(z).$$

There are three singularities  $0, 1, \infty$ , and are all regular.

Since the residues at  $z = 0$  and  $z = 1$  are the variables  $x_0$  and  $x_1$  up to sign, one can think of this differential equation as a “universal” first order differential equation with regular singularities at  $0, 1, \infty$ .

Near  $0$ , we have

$$\sum_{m \geq 0} \frac{1}{m!} (\log z)^m x_0^m = e^{x_0 \log z}.$$

Initial condition:

$$\lim_{z \rightarrow 0} \widehat{\text{Li}}(z) e^{-x_0 \log z} = 1.$$

Near  $1$ , we have

$$\lim_{z \rightarrow 1} e^{-x_1 \log(1-z)} \widehat{\text{Li}}(z) = \phi_{KZ}(x_0, x_1).$$

This is the associator of Knizhnik-Zamolodchikov, introduced by Drinfeld.

We can study the monodromy of the differential equation. Minh and Petitot proved:

**Theorem.**  $\{\widehat{\text{Li}}_w(z)\}_{w \in X^*}$  are linearly independent over  $\mathbb{R}(z)$ .

# Introduction to Multiple Zeta Values, IV

M. WALDSCHMIDT

*August 25, 2001*

**Conjectural description of  $\ker \hat{\zeta}$ .** We first review the known linear relations among zeta values. Take  $u, v \in \mathcal{H}^0$  (with  $k = \mathbb{Q}$ ), then

$$\hat{\zeta}(u * v - u \text{ III } v) = 0.$$

PROOF.  $\hat{\zeta}(u) \cdot \hat{\zeta}(v) = \hat{\zeta}(u * v) = \hat{\zeta}(u \text{ III } v)$ . ■

We also have the following relation, due to Euler:

$$\zeta(3) = \zeta(2, 1).$$

Therefore,  $y_3 - y_2 y_1 \in \ker \hat{\zeta}$ . But the preceding system of relations all have weights  $\geq 4$ . So Euler's relation is not spanned by the previous ones.

We have

$$\begin{aligned} x_1 * (x_0 x_1) &= y_1 * y_2 = y_1 y_2 + y_2 y_1 + y_3, \\ x_1 \text{ III } (x_0 x_1) &= 2x_0 x_1^2 + x_1 x_0 x_1. \end{aligned}$$

Notice that  $x_1 \notin \mathcal{H}^0$ . Still, the above computation suggests that

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

However,  $\zeta(1, 2)$  is not well-defined. If it were, we would have got Euler's relation legitimately.

We have (from Chen integrals)

$$\text{Li}_1(z) \cdot \text{Li}_2(z) = \text{Li}_{x_1 \text{ III } x_0 x_1}(z) = 2 \text{Li}_{2,1}(z) + \text{Li}_{1,2}(z),$$

valid for  $|z| < 1$ . If we look at the series,

$$\begin{aligned} \text{Li}_1(z) \cdot \text{Li}_2(z) &= \sum_{n \geq 1} \frac{z^n}{n} \sum_{m \geq 1} \frac{z^m}{m^2} \\ &= \sum_{n > m} \frac{z^n z^m}{n m^2} + \sum_{m > n} \frac{z^n z^m}{n m^2} + \sum_{n=m} \frac{z^{2n}}{n^3} \\ &= \text{Li}_{1,2}(z, z) + \text{Li}_{2,1}(z, z) + \text{Li}_3(z^2). \end{aligned}$$

Here, we have used

**Definition.**

$$\text{Li}_{\underline{s}}(z_1, \dots, z_k) = \sum_{n_1 > \dots > n_k \geq 1} \frac{z_1^{n_1} \dots z_k^{n_k}}{n_1^{s_1} \dots n_k^{s_k}}.$$

We now have

$$\text{Li}_3(z^2) - 2 \text{Li}_{2,1}(z) + \text{Li}_{2,1}(z, z) = \text{Li}_{1,2}(z, 1) - \text{Li}_{1,2}(z, z).$$

The LHS is  $\zeta(3) - \zeta(2, 1)$  when  $z = 1$ . It is an exercise that  $\lim_{z \rightarrow 1} \text{RHS} = 0$ .

This proves the Euler relation, which is an example of *the third standard relations*:

$$\zeta(x_1 * w - x_1 \amalg w) = 0 \quad \text{for all } w \in \mathcal{H}^0.$$

**Algebraic relations among zeta values.**

*Linear relations*  $\leftrightarrow \ker \hat{\zeta}$ .

**Conjecture 1.** (Hoffman).  $\ker \hat{\zeta}$  is spanned by elements in  $\mathcal{H}^0$  homogeneous for weight.

Denote by  $\mathcal{Z}_p$  the  $\mathbb{Q}$ -space spanned by  $\hat{\zeta}(w)$ ,  $w \in \mathcal{H}_p^0$  (homogeneous elements in  $\mathcal{H}^0$  of weight  $p$ ).

Conjecture 1 implies that the  $\mathbb{Q}$ -algebra spanned by  $\mathcal{Z}_p$ ,  $p \geq 0$  is  $\bigoplus_{p \geq 0} \mathcal{Z}_p$ . That is, all algebraic relations are given by homogeneous relation. This statement was conjectured by Goncharov.

We have:

$$\begin{aligned} \mathcal{Z}_0 &= \mathbb{Q}, \\ \mathcal{Z}_1 &= 0, \\ \mathcal{Z}_2 &= \langle \zeta(2) \rangle_{\mathbb{Q}} = \langle \pi^2 \rangle, \\ \mathcal{Z}_3 &= \langle \zeta(3) \rangle_{\mathbb{Q}}, \\ \mathcal{Z}_4 &= \langle \zeta(4) \rangle_{\mathbb{Q}} = \langle \pi^4 \rangle_{\mathbb{Q}}, \\ \mathcal{Z}_5 &= \langle \zeta(2)\zeta(3), \zeta(5) \rangle_{\mathbb{Q}}. \end{aligned}$$

So if we put  $d_p = \dim \mathcal{Z}_p$ , we have  $d_1 = 0$ ,  $d_0 = d_2 = d_3 = d_4 = 1$ ,  $1 \leq d_5 \leq 2$ . We do not know whether  $\zeta(2)\zeta(3)/\zeta(5) \in \mathbb{Q}$ .

There is a program for finding relations, called “EZ-face”, available on the internet

<http://www.cecm.sfu.ca/projects/EZFace/index.html>

*Exercise.*  $\zeta(3, 1) = \frac{1}{4}\zeta(4)$ ,  $\zeta(2, 2) = \frac{3}{4}\zeta(4)$ ,  $\zeta(2, 1, 1) = \zeta(4)$ .

**Conjecture.** (Zagier). For all  $p \geq 0$ ,  $d_p = d_{p-2} + d_{p-3}$ . Hence

$$\sum_{p \geq 0} d_p t^p = \frac{1}{1 - t^2 - t^3}.$$

The “exercise” of checking the compatibility of conjectures of Zagier and Goncharov is not an easy one, and has not yet been done completely.

The number of  $\zeta(\underline{s})$  of weight  $s_1 + \dots + s_k = p$  (with  $s_1 \geq 2$ ) is  $2^{p-2}$ .

The number of linear relations is  $2^{p-5}(p+1)$ . Here we are not counting independent relations just the ways of getting relations. It is not easy to see what are the independent linear relations among these relations.

Each  $\zeta(\underline{s})$  with  $|\underline{s}| \leq 11$  are homogeneous polynomials in

$$\zeta(2), \zeta(3), \zeta(5), \zeta(7), \zeta(9), \zeta(11), \zeta(6, 2), \zeta(8, 2), \zeta(8, 2, 1).$$

Broadhurst has given a conjectural description for such a list for  $|\underline{s}| \leq p$ . (This is a problem in algebra).

*Suggestion of Hoffman.* A basis for  $\mathcal{Z}_p$  may be

$$\zeta(s_1, \dots, s_k), \quad s_j \in \{2, 3\}.$$

**Conjecture.** The three standard relations (shuffle, stuffle, and the third, which are respectively quadratic, quadratic, and linear) generate the ideal of all algebraic relations among zeta values.

More precisely, take independent variables  $\mathcal{Z}_{\underline{s}}$ ,  $\underline{s} = (s_1, \dots, s_k)$  with  $s_1 \geq 2$  and consider the map  $\mathbb{Q}[\mathcal{Z}_{\underline{s}} : s_1 \geq 2] \rightarrow \mathbb{R}$ ,  $\mathcal{Z}_{\underline{s}} \mapsto \zeta(\underline{s})$ . Then the conjecture is that the kernel of this map is the ideal spanned by

$$Z_u Z_v - Z_{u \amalg v}, \quad Z_u Z_v - Z_{u * v}, \quad Z_{x_1 * w} - x_1 \amalg w,$$

where  $u, v, w \in \mathcal{H}^0$ , and  $Z_u$  means  $\mathcal{Z}_{\underline{s}}$  if  $u = y_{\underline{s}}$ .

*Consequence(?).*  $\pi, \zeta(3), \zeta(5), \dots$  are algebraically independent.

*Other relations.* Is it true that  $\hat{\zeta}(u * v - u \amalg v) = 0$  with  $u, v \in \mathcal{H}^1$  but  $u * v - u \amalg v \in \mathcal{H}^0$ ? The answer is no. There exist  $u, v \in \mathcal{H}^1$  such that  $u * v - u \amalg v \in \mathcal{H}^0$  but  $\zeta(u * v - u \amalg v) \neq 0$ .

*Example.*  $u = x_1, v = x_1, u \amalg v = 2x_1^2$  and  $u * v = x_1 * x_1 = y_1 * y_1 = 2y_1^2 + y_2 = 2x_1^2 + y_2$ . Therefore,  $u * v - u \amalg v = y_2 \in \mathcal{H}^0$  but  $\zeta(y_2) = \zeta(2) \neq 0$ .

The map  $\hat{\zeta} : \mathcal{H}^0 \rightarrow \mathbb{R}$  is a morphism of algebras for  $*$  and  $\amalg$ . We want to extend it to  $\mathcal{H}^1$ . If  $\hat{\zeta} : \mathcal{H}^1 \rightarrow \mathbb{R}$  were a morphism for  $*$  and  $\amalg$ , we would have

$$\hat{\zeta}(x_1)^2 = \hat{\zeta}(x_1 * x_1) = \hat{\zeta}(x_1 \amalg x_1).$$

But the 2nd equality is not true.

# Introduction to Multiple Zeta Values, V

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**Extension of  $\hat{\zeta}$  to  $\mathcal{H}^1 \supset \mathcal{H}^0$ .** Recall that

$$\mathcal{H} = \mathbb{Q}\langle x_0, x_1 \rangle \quad \supset \quad \mathcal{H}^1 = \mathbb{Q}.e + \mathcal{H}.x_1 \quad \supset \quad \mathcal{H}^0 = \mathbb{Q}.e + x_0.\mathcal{H}.x_1.$$

Also, recall that  $\hat{L}i_w(z)$  is defined for  $w \in \mathcal{H}^1$ , and  $\hat{\zeta}(w)$  is defined for  $w \in \mathcal{H}^0$ .

We also have

$$\mathcal{H}_{\text{III}} = \mathbb{Q}[\mathcal{L}]_{\text{III}} \quad \supset \quad \mathcal{H}_{\text{III}}^1 = \mathbb{Q}[\mathcal{L} \setminus \{x_0\}]_{\text{III}} \quad \supset \quad \mathcal{H}_{\text{III}}^0 = \mathbb{Q}[\mathcal{L} \setminus \{x_0, x_1\}]_{\text{III}}.$$

Also  $\hat{\zeta} : \mathcal{H}_{\text{III}}^0 \rightarrow \mathbb{R}$  and  $\mathcal{H}_{\text{III}}^1 = \mathcal{H}_{\text{III}}^0[x_1]$ . So we only have to decide what  $\zeta(1)$  is. The difficulty is that  $\zeta(1)$  is not defined (possible candidates: 0 or the Euler constant  $\gamma$ ). An easy way out, since there are more than one reasonable choices, is to make no choice:

Denote by  $\hat{Z}_{\text{III}}$  the unique morphism of algebras  $\mathcal{H}_{\text{III}}^1 \rightarrow \mathbb{R}[T]$  such that  $\hat{Z}_{\text{III}}(w) = \hat{\zeta}(w)$  for  $w \in \mathcal{H}_{\text{III}}^0$ , and  $\hat{Z}_{\text{III}}(x_1) = T$ , where  $T$  is an indeterminate. We do the same with  $\mathcal{H}_*$ . We have

$$\hat{Z}_* : \mathcal{H}_*^1 \rightarrow \mathbb{R}[T], \quad x_1 \mapsto T.$$

**Theorem.** (Boutet de Mouvel, Zagier). There is an isomorphism of  $\mathbb{R}$ -vector spaces  $\rho : \mathbb{R}[T] \rightarrow \mathbb{R}[T]$  such that

$$\begin{array}{ccc} & & \mathbb{R}[T] \\ & \nearrow \hat{Z}_{\text{III}} & \uparrow \rho \\ \mathcal{H}^1 & & \mathbb{R}[T] \\ & \searrow \hat{Z}_* & \end{array}$$

is commutative.

In fact,  $\rho$  is determined by the formula:

$$\sum_{\ell \geq 0} \frac{1}{\ell!} \rho(T^\ell) t^\ell = \exp\left(Tt + \sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} t^n\right)$$

explicit formula is more interesting.

*Example.*  $\rho(T^0) = 1$ ,  $\rho(T) = T$ ,  $\rho(T^2) = T^2 + \zeta(2)$ ,  $\rho(T^3) = T^3 + 3\zeta(2)T - 2\zeta(3)$ ,  $\rho(T^4) = T^4 - 6\zeta(2)T^2 - 8\zeta(3)T + 6\zeta(4) + 3\zeta(2)^2$ .

We can check:  $x_1 \text{ III } x_1 = 2x_1^2$ , so  $\hat{Z}_{\text{III}}(2x_1^2) = T^2$ . On the other hand,  $x_1 * x_1 = 2x_1^2 + x_2$ . So  $\hat{Z}_*(2x_1^2) = T^2 - \zeta(2)$ .



We have for  $s \geq 2$ ,

$$\exp\left(\sum_{n=1}^{\infty} (-1)^n \frac{t^n}{n} \zeta(sn)\right) = \prod_{j \geq 1} \left(1 + \frac{t}{j^s}\right)^{-1}.$$

The RHS reminds us of the product formula for  $\Gamma$ -function. In fact, we should compare the above with

$$\exp\left(-\gamma t + \sum_{n=2}^{\infty} (-1)^n \frac{t^n}{n} \zeta(sn)\right) = \Gamma(1+t).$$

We also have

$$\rho(e^{Tt}) = e^{Tt} \cdot \exp\left(\sum_{n \geq 2} (-1)^n \frac{\zeta(n)}{n} t^n\right).$$

So we can consider  $\rho$  as a differential operator

$$\rho = \exp\left(\sum_{n \geq 2} (-1)^n \frac{\zeta(n)}{n} \left(\frac{\partial}{\partial T}\right)^n\right).$$

*Hint for the proof of Zagier-Boutet de Monvel.* Recall

$$\mathcal{H}_*^1 \xrightarrow{\sim} Q \text{ Sym}, \quad y_{\underline{s}} \mapsto QM_{\underline{s}}(\underline{t}) = \sum_{n_1 > \dots > n_k \geq 1} t_{n_1}^{s_1} \dots t_{n_k}^{s_k}.$$

The specialization  $t_n = 1/n$ ,  $n \geq 1$  gives  $\hat{\zeta}$  on  $\mathcal{H}^0$ .

Take  $N$  large and consider the specialization  $\underline{t} \mapsto (1, 1/2, 1/3, \dots, 1/N, 0, \dots)$ , we get asymptotic expansions. Moreover, consider

$$\begin{aligned} \exp_{\text{III}}(ty_1) &= \sum_{n \geq 0} \frac{t^n}{n!} y_1^{\text{III}n} = \sum_{n \geq 0} t^n y_1^n, \\ \exp_*(ty_1) &= \sum_{n \geq 0} \frac{t^n}{n!} y_1^{*n}. \end{aligned}$$

We then use Newton's formulae.

*Next step.* From  $\mathcal{H}^1$  to  $\mathcal{H}$ . We will extend the map

$$\hat{\zeta}_{\text{III}} : \mathcal{H}_{\text{III}}^1 \rightarrow \mathbb{R}[T] \xrightarrow{\text{Ty}_0} \mathbb{R}$$

to  $\mathcal{H}_{\text{III}}$ . Recall that  $\mathcal{H}_{\text{III}} = \mathcal{H}_{\text{III}}^0[x_0, x_1]$  (commutative polynomial algebra). So given  $w \in \mathcal{H}_{\text{III}}$ , we can associate the constant term (as a polynomial in  $x_0, x_1$ ) in  $\mathcal{H}_{\text{III}}^0$ . Call this map  $\text{Reg}_{\text{III}} : \mathcal{H}_{\text{III}} \rightarrow \mathcal{H}_{\text{III}}^0$  (the notation means: regularize a possibly non-convergent word to a convergent word). We now define

$$\hat{\zeta}_{\text{III}} = \hat{\zeta} \circ \text{Reg}_{\text{III}} : \mathcal{H}_{\text{III}} \rightarrow \mathbb{R}.$$

**Proposition.** (K. Ihara and M. Kaneko). Let  $w \in X^*$ ,  $w = x_1^m w_0 x_0^n$  with  $w_0 \in \mathcal{H}^0$ . Then

$$\text{reg}_{\text{III}}(w) = \sum_{i=0}^m \sum_{j=0}^n (-1)^{i+j} x_1^i \text{III} (x_1^{m-i} w_0 x_0^{n-j}) \text{III} x_0^j.$$

Moreover,

$$w = \sum_{i=0}^m \sum_{j=0}^n \text{Reg}_{\text{III}}(x_1^{m-i} w_0 x_0^{n-j}) \text{III} x_1^i \text{III} x_0^j.$$

*Examples.*  $\text{Reg}_{\text{III}}(x_0^n) = \text{Reg}_{\text{III}}(x_1^m) = 0$  for  $n \geq 1, m \geq 1$ . Also  $\text{Reg}_{\text{III}}(x_1^m x_0^n) = (-1)^{n+m-1} x_0^n x_1^m$ .

**Theorem.** (Ihara and Kaneko). For  $w \in \mathcal{H}^1$  and  $w_0 \in \mathcal{H}^0$ ,

$$\text{reg}_{\text{III}}(w * w_0 - w \text{III} w_0) \in \ker \hat{\zeta}.$$

That is,  $\hat{\zeta}_{\text{III}}(w * w_0 - w \text{III} w_0) = 0$ .

**Conjecture.** (Ihara and Kaneko) As a  $\mathbb{Q}$ -vector space,  $\ker \hat{\zeta}$  is spanned by these elements.

The third standard relations can be obtained from  $w * w_0 - w \text{III} w_0$  by taking  $w = x_1$ . In general, we must regularize. This conjecture is probably more reasonable (more generators for the kernel), but is perhaps equivalent to the previous conjecture.

*Example.*  $x_1^2 * x_0 x_1 - x_1^2 \text{III} x_0 x_1 = x_1 x_0 x_1^2 - x_1 x_0^2 x_1 - x_0^2 x_1^2$  is not in  $\mathcal{H}^0$ .

*(Esterlé shows: The conjecture of Ihara and Kaneko is equivalent to the following:  $\ker \hat{\zeta}$  is spanned by*

$$w_1 * w_2 - w_1 \text{III} w_2, \text{ with } w_1, w_2 \in \mathcal{H}^0$$

and

$$\text{Reg}_{\text{III}}(x_1^m * w_0 - x_1^m \text{III} w_0) \text{ with } w_0 \in \mathcal{H}^0 \text{ and } m \geq 1.$$

For each  $m \geq 1$ , consider the map

$$\theta_m : \mathcal{H} \rightarrow \mathcal{H}, \quad m \mapsto (-1)^m \text{Reg}_{\text{III}}(x_1^m * w - x_1^m \text{III} w).$$

- For  $w_0 \in \mathcal{H}^0$ , it is known that  $\theta_m(w_0) \in \ker(\hat{\zeta})$ .
- For  $m = 1$ ,  $w \mapsto x_1 \text{III} w - x_1 * w$  (no need to regularize).
- $\text{Reg}_{\text{III}}(x_1^m) = 0 \implies \theta_m(w) = (-1)^m \text{Reg}_{\text{III}}(x_1^m * w)$ .

**Definition.** We define  $\hat{\zeta}_*$  as  $\hat{\zeta} \circ \text{Reg}_*$ , where  $\text{Reg}_* : \mathcal{H}_* = \mathcal{H}_*[x_0, x_1] \rightarrow \mathcal{H}_*$  is again “taking the constant term”.

We have

$$\text{Reg}_*(x_1^m w_0) = \sum_{i=0}^m (-1)^i \frac{x_1^{*i}}{i!} * (x_1^{m-i} w_0)$$

for  $w_0 \in \mathcal{H}^0$ .

**Other linear relations on the multiple zeta values.**

*Duality.* Start with

$$\int_{x_0}^{x_1} \varphi_1 \cdots \varphi_p = \int_{x_1 > t_1 > \cdots > t_p > x_0} \varphi_1(t_1) \cdots \varphi_p(t_p) = \int_{x_1}^{x_0} \varphi_p \cdots \varphi_1(-1)^p.$$

So

$$\int_0^1 \omega_{\epsilon_1} \cdots \omega_{\epsilon_p} = \int_0^1 \omega_{1-\epsilon_p} \cdots \omega_{1-\epsilon_1}.$$

Denote  $(1, \dots, 1)$  ( $\ell$  times) by  $\{1\}_\ell$ . Write

$$\underline{s} = (s_1, \dots, s_k) = (t_1 + 2, \{1\}_{r_1}, t_2 + 2, \{1\}_{r_2}, \dots, t_m + 2, \{1\}_{r_m})$$

with  $t_1, \dots, t_m, r_1, \dots, r_m \geq 0$ . Let  $\tau : \mathcal{H} \rightarrow \mathcal{H}$  be the anti-isomorphism exchanging  $x_0$  and  $x_1$ . Then  $\tau y_{\underline{s}} = y_{\underline{s}'}$  where  $\underline{s}' = (r_m + 2, \{1\}_{t_m}, \dots, r_1 + 2, \{1\}_{t_1})$ . The duality relation is:

$$\zeta(\tau y_{\underline{s}}) = \zeta(y_{\underline{s}}).$$

# Introduction to Multiple Zeta Values, VI

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Recall that we have

$$\begin{array}{c}
 \mathcal{H} = \mathbb{Q}\langle x_0, x_1 \rangle \\
 \parallel \\
 \mathcal{H}^1 = \mathbb{Q}.e + \mathcal{H}.x_1 \\
 \parallel \\
 \mathcal{H}^0 = \mathbb{Q}.e + x_0.\mathcal{H}.x_1 \xrightarrow{\hat{\zeta}} \mathbb{R}
 \end{array}$$

$\ker \hat{\zeta} \leftrightarrow$  linear dependence relations among multiple zeta values.

We have the basic *double shuffle relations*:

$$\begin{aligned}
 \hat{\zeta}(u)\hat{\zeta}(v) &= \hat{\zeta}(u \text{ III } v) = \hat{\zeta}(u * v) \quad \text{for all } u, v \in \mathcal{H}^0, \\
 &\implies u \text{ III } v - u * v \in \ker \hat{\zeta}.
 \end{aligned}$$

Ihara and Kaneko give the more general *regularized double shuffle relations*:

$$\text{(RDSR)} \quad \text{Reg}_{\text{III}}(w \text{ III } w_0 - w * w_0) \in \ker \hat{\zeta}, \quad w_0 \in \mathcal{H}^0, w \in \mathcal{H}^1,$$

where

$$\text{Reg}_{\text{III}} : \mathcal{H} = \mathcal{H}^0[x_0, x_1]_{\text{III}} \rightarrow \mathcal{H}^0$$

sends a polynomial to its constant term.

*Remark.*

- For  $w = x_1$ ,  $x_1 \text{ III } w_0 - x_1 * w_0 = d_1(w_0) \in \mathcal{H}^0$  for  $w_0 \in \mathcal{H}^0$ , there is no need to regularize.
- For  $w = x_1^n$ ,  $n \geq 1$ , RDSR can be written as

$$\sum_{i=0}^n (-1)^i x_1^i \text{ III } (x_1^{n-i} * w_0) \in \ker \hat{\zeta}.$$

- The function  $d_1 : \mathcal{H}^0 \rightarrow \mathcal{H}^0$  above is the derivation (satisfying  $d(uv) = udv + (du)v$ ) on  $\mathcal{H}$  with  $d_1(x_0) = x_0x_1$ ,  $d_1(x_1) = -x_0x_1$ . We have

$$d_1(x_0^{s-1}x_1) = \sum_{i=1}^{s-1} x_0^i x_1 x_0^{s-1-i} x_1 - x_0^s x_1.$$

– Consequence of  $d_1(y_s) \in \ker \hat{\zeta}$ :

$$(Euler) \quad \zeta(s+1) = \sum_{i=1}^{s-1} \zeta(i+1, s-i).$$

This is a special case of the more general *sum formula*: for  $p \geq k+1$ ,  $k \geq 1$  fixed,

$$\sum_{\underline{s}=(s_1, \dots, s_k): s_1 + \dots + s_k = p} \zeta(\underline{s}) = \zeta(p).$$

This reduces to Euler's relation when  $k=2$ . For  $k=3$ , it was proved by Hoffman and Moen (1996). The general formula for  $k \geq 2$  is due to Granville-Zagier (1997). They were often first observed numerically on computers.

*Examples.*

- $\zeta(3) = \zeta(2, 1)$ , and more generally,
- $\zeta(2, \{1\}_{k-1}) = \zeta(k+1)$  (take  $p = k+1$  in the sum formula).

*Proof of the sum formula from RDSR.* Granville-Zagier proved the formula by analytic means. We would like to see how to get the formula from RDSR.

For  $m \geq 0$ ,  $w \in \mathcal{H}$ , let

$$\theta_m(w) = (-1)^m \text{Reg}_{\text{III}}(x_1^m * w).$$

So  $\theta_m(w) \in \ker \hat{\zeta}$  for  $m \geq 1$ ,  $w \in \mathcal{H}^0$ .

**Lemma.** (Ihara-Kaneko) For  $p > k+1$ ,  $k \geq 1$ ,

$$\theta_k(x_0^{p-k-1} x_1) = x_0(x_1^k \text{III } x_0^{p-k-2})x_1 - x_0(x_1^{k-1} \text{III } x_0^{p-k-1})x_1.$$

The proof is just a simple induction.

The expression  $x_1^{k-1} \text{III } x_0^{p-k-1}$  is of length  $k-1$  and weight  $p-2$  (recall that the length is the number of  $x_1$ 's, and the weight is the number of letters). Let

$$S(p, k) = x_0(x_1^{k-1} \text{III } x_0^{p-k-1})x_1.$$

This is the sum of all convergent words of length  $k$  and weight  $p$ . Thus

$$\theta_k(x_0^{p-k-1} x_1) = S(p, k+1) - S(p, k) \in \ker \hat{\zeta}, \quad 1 \leq k < p-1.$$

It follows that  $S(p, k) - S(p, 1) \in \ker \hat{\zeta}$ , for  $1 \leq k \leq p-1$ . But  $S(p, 1)$  is just  $x_0^{p-1} x_1$ , so  $\hat{\zeta}(S(p, 1)) = \zeta(p)$ . On the other hand,

$$\hat{\zeta}(S(p, k)) = \sum_{s_1 \geq 2, s_1 + \dots + s_k = p} \zeta(s_1, \dots, s_k).$$

This proves the sum formula.

**Ohno's relations.** These contain all the relations given earlier.

Let's first recall the duality relation: let  $\tau : \mathcal{H} \rightarrow \mathcal{H}$  be the anti-automorphism exchanging  $x_0$  and  $x_1$  (anti-automorphism means that  $\tau(uv) = \tau(v)\tau(u)$ ). Then  $(1 - \tau)w_0 \in \ker \hat{\zeta}$  for  $w \in \mathcal{H}^0$ ; this follows from the identity

$$\int_0^1 \omega_0^{t_1+1} \omega_1^{r_1+1} \dots \omega_0^{t_m+1} \omega_1^{r_m+1} = \int_0^1 \omega_0^{r_m+1} \omega_1^{t_m+1} \dots \omega_0^{r_1+1} \omega_1^{t_1+1}$$

which can be checked by a change of variables. Fix  $\underline{s} = (s_1, \dots, s_k)$  and  $\ell \geq 0$ . Write  $\tau y_{\underline{s}} = y_{\underline{s}'}$ ,  $\underline{s}' = (s'_1, \dots, s'_{k'})$ . Then Ohno's relation is

$$\sum_{e_1 + \dots + e_k = \ell, e_i \geq 0} \zeta(s_1 + e_1, \dots, s_k + e_k) = \sum_{e'_1 + \dots + e'_{k'} = \ell, e'_j \geq 0} \zeta(s'_1 + e'_1, \dots, s'_{k'} + e'_{k'}).$$

This contains the duality relation: just set  $\ell = 0$ . It also contains the sum relation, which is

$$\zeta(p) = \sum_{|\underline{\sigma}|=p, \text{length}(\underline{\sigma})=h} \zeta(\underline{\sigma}).$$

We can take  $k = 1, s_1 = h + 1, e = p - h - 1$ .

*Ihara-Kaneko:* Ohno's formula is equivalent to: for  $n \geq 1, w \in \mathcal{H}^0, d_n(w) \in \ker \hat{\zeta}$ , where  $d_n$  is the derivation on  $\mathcal{H}$  such that

$$\begin{aligned} d_n(x_0) &= x_0(x_0 + x_1)^{n-1} x_1, \\ d_n(x_1) &= -x_0(x_0 + x_1)^{n-1} x_1. \end{aligned}$$

Notice that  $(x_0 + x_1)^{n-1}$  is the sum of all monomials of weight  $n - 1$ , and  $d_n(x_0)$  is the sum of all monomials of weight  $n + 1$  in  $\mathcal{H}^0$ .

People are working on deriving Ohno's relation from RDSR.

**A conjecture of Zagier.** The conjecture was given in 1994, and solved by Borwein in 1997. Bradley and Minh-Petitot (2000) proved it using syntactic identities:

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

*Definition.* For  $S \in \mathbb{Q}\langle\langle x_0, x_1 \rangle\rangle$  such that  $(S|e) = 0$ ,

$$S^* = e + S + S^2 + \dots$$

is the unique solution to either  $(1 - S)S^* = e$  or  $S^*(1 - S) = e$ . We have  $(y_2^*) * (-y_2)^* = (-y_4)^*$ .

*Idea of proof:* consider  $\mathcal{H}_*^0 \xrightarrow{\sim} Q\text{Sym}^0$ , sending  $y_{\underline{s}}$  to

$$QM(\underline{s}) = \sum_{n_1 > \dots > n_k \geq 1} t_{n_1}^{s_1} \dots t_{n_k}^{s_k}$$

and

$$\sum_{n_1 > \dots > n_k \geq 1} t_{n_1}^2 \dots t_{n_k}^2 = \prod_{n \geq 1} (1 + t_n^2) \longleftrightarrow y_2^*.$$

So the formula  $y_2^* * (-y_2)^* = -y_4^*$  amounts to

$$\prod (1 + t_n^2) \prod (1 - t_n^2) = \prod (1 - t_n^4).$$

$$(1) \quad (x_0 x_1)^* \text{ III } (-x_0 x_1)^* = (-4x_0^2 x_1^2)^*.$$

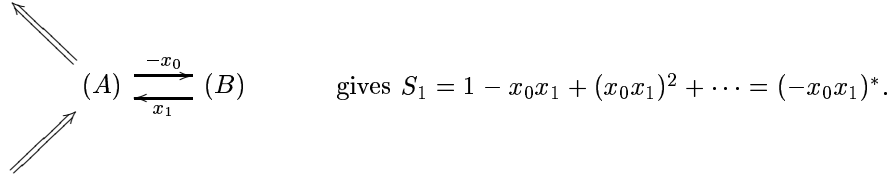
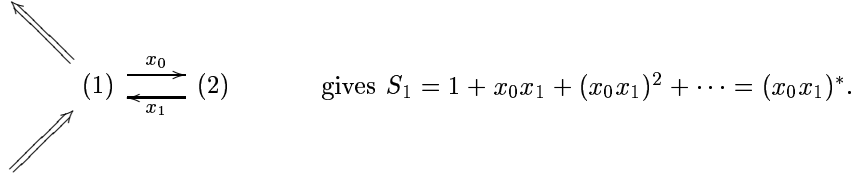
We replace  $x_0$  by  $t\omega_0 = tdz/z$ ,  $x_1$  by  $t\omega_1 = tdz/(1-z)$ . We get

$$\int_0^1 (-t^4 \omega_0^3 \omega_1)^* = \sum_{k \geq 0} (-t)^{4k} \zeta(\{4\}_k).$$

$$\int_0^1 (-4t^4 \omega_0^2 \omega_1^2)^* = \sum_{k \geq 0} (-4t^4)^k \zeta(\{3, 1\}_k).$$

Thus Zagier's relation is that the difference of the LHS's is in the kernel of  $\hat{\zeta}$ .

*Example.* Consider the following automaton:



**Values of  $\text{Li}_s(\underline{z})$  at roots of unity.** Say we consider  $N$ -th roots of unity.

When  $N = 1$ , this is the classical theory of multiple zeta values. We have Zagier's conjecture on the dimension spanned by zeta values:

$$d_p = d_{p-2} + d_{p-3}.$$

When  $N = 2$ ,

$$d_p = d_{p-1} + d_{p-2}.$$

When  $N = 3$ ,

$$d_p = 2^p.$$

$N = 4$ , complicated...

*Half integers.* For example,

$$\begin{aligned}\operatorname{Li}_2(1/2) &= \frac{\pi^2}{12} - \frac{1}{2}(\log 2)^2, \\ \zeta(3) &= \frac{1}{12}\pi^2 \log 2 + \operatorname{Li}_{(2,1)}(1/2) + \operatorname{Li}_3(1/2).\end{aligned}$$

This last formula is due to Ramanujan:

$$\sum_{n=1}^{\infty} \frac{1}{2^n n^2} \sum_{j=1}^n \frac{1}{j} = \zeta(3) - \frac{1}{12}\pi^2 \log 2.$$

*Generalized Hurwitz zeta function.*

$$\sum_{n_1 > \dots > n_k \geq 1} \frac{z_1^{n_1}}{(n_1 - t_1)^{s_1}} \cdots \frac{z_k^{n_k}}{(n_k - t_k)^{s_k}}.$$

What about the transcendence of  $\zeta(1/2)$  or  $\zeta(i)$ ? The solution may not have immediate consequence but certainly requires new ideas.

<http://www.institut.math.jussieu.fr/~miw/articles/ps/ncts.ps>

<http://math.cts.nthu.edu.tw/Mathematics/english/lecture.html>

*see also:*

<http://www.institut.math.jussieu.fr/~miw//articles/ps/mpl.ps>