## Number Theory

# Multiple polylogarithm values at roots of unity 

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#### Abstract

For any positive integer $N$ let $\mu_{N}$ be the group of the $N$ th roots of unity. In this note we shall study the $\mathbb{Q}$-linear relations among the values of multiple polylogarithms evaluated at $\boldsymbol{\mu}_{N}$. We show that the standard relations considered by Racinet do not provide all the possible relations in the following cases: (i) level $N=4$, weight $w=3$ or 4, and (ii) $w=2,7<N<50$, and $N$ is a power of 2 or 3 , or $N$ has at least two prime factors. We further find some (presumably all) of the missing relations in (i) by using the octahedral symmetry of $\mathbb{P}^{1}-\left(\{0, \infty\} \cup \boldsymbol{\mu}_{4}\right)$. We also prove some other results when $N=p$ or $N=p^{2}(p$ prime $\geqslant 5)$ by using the motivic fundamental group of $\mathbb{P}^{1}-\left(\{0, \infty\} \cup \mu_{N}\right)$. To cite this article: J. Zhao, C. R. Acad. Sci. Paris, Ser. I 346 (2008). © 2008 Académie des sciences. Published by Elsevier Masson SAS. All rights reserved.


## Résumé

Valeurs de polylogarithmes multiples en des racines de l'unité. Soient $N$ un entier positif et $\boldsymbol{\mu}_{N}$ le groupe des racines $N$ ièmes de l'unité. Nous étudions les relations $\mathbb{Q}$-linéaires entre les valeurs de polylogarithmes multiples évalués en ces racines de l'unité. Nous montrons que les relations standard considérées par Racinet ne fournissent pas toutes les relations dans les cas suivants : (i) $N=4$, poids $w=3$ ou 4 , et (ii) $w=2,7<N<50$, et $N$ est une puissance de 2 ou 3 , ou $N$ a au moins deux facteurs premiers. Dans le cas (i), nous trouvons des (sans doute, toutes les) relations manquantes à l'aide de la symétrie octaédrale de $\mathbb{P}^{1}-\left(\{0, \infty\} \cup \mu_{4}\right)$. Utilisant le groupe fondamental motivique de $\mathbb{P}^{1}-\left(\{0, \infty\} \cup \boldsymbol{\mu}_{N}\right)$, nous obtenons des résultats additionnels quand $N=p$ ou $N=p^{2}(p$ premier $\geqslant 5)$. Pour citer cet article : J. Zhao, C. R. Acad. Sci. Paris, Ser. I 346 (2008). © 2008 Académie des sciences. Published by Elsevier Masson SAS. All rights reserved.

## 1. Introduction

Double shuffle relations have played significant roles in the study of multiple zeta values in recent years. These relations can be easily generalized to multiple polylogarithm values at roots of unity (MPVs):

$$
\begin{equation*}
L i_{s_{1}, \ldots, s_{n}}\left(\zeta_{1}, \ldots, \zeta_{n}\right):=\sum_{k_{1}>\cdots>k_{n}>0} \frac{\zeta_{1}^{k_{1}} \cdots \zeta_{n}^{k_{n}}}{k_{1}^{s_{1}} \cdots k_{n}^{s_{n}}}, \quad\left(s_{1}, \zeta_{1}\right) \neq(1,1), \tag{1}
\end{equation*}
$$

where $\zeta_{j}$ 's run through $N$ th roots of unity. We call $N$ the level and $w:=s_{1}+\cdots+s_{n}$ the weight. One major problem is to determine the dimension $d(w, N)$ of the $\mathbb{Q}$-vector space $\mathcal{M} \mathcal{P} \mathcal{V}(w, N)$ spanned by these values.

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In [7], Racinet listed the following relations: double shuffle relations and their regularized versions (by regularizing both the divergent integrals and divergent series representing MPVs), (regularized) distributions, and weight one relations. We can also add the lifted relations obtained by multiplying the above relations by any MPV and then expanding all the products by shuffle relations (see [8]). We will call these standard relations. By intensive MAPLE computation it is shown [8] that in many cases these relations cannot produce all the possible $\mathbb{Q}$-linear relations. For example, standard relations imply only $d(3,4) \leqslant 9$ which is one more than the bound given by [4, 5.25]. Concretely, from standard relations MAPLE confirms the following

Fact: Every MPV of weight 3 and level 4 can be written explicitly
as a linear combination of the nine MPVs appearing in (2),
and no further $\mathbb{Q}$-linear relations between these values can be deduced from the standard relations. But by GiNac [6] and EZface [1] the following is found numerically (see [8, Remark 10.1])

$$
\begin{align*}
5 L i_{1,2}(-1,-i)= & 46 L i_{1,1,1}(i, 1,1)-7 L i_{1,1,1}(-1,-1, i)-13 L i_{1,1,1}(i, i, i)+13 L i_{1,2}(-i, i) \\
& -L i_{1,1,1}(-i,-1,1)+25 L i_{1,1,1}(-i, 1,1)-8 L i_{1,1,1}(i, i,-1)+18 L i_{2,1}(-i, 1) \tag{2}
\end{align*}
$$

In this note, we shall prove (2) by the explicit relations in $(*)$ using the octahedral symmetry of $\mathbb{P}^{1}-\left(\{0, \infty\} \cup \mu_{4}\right)$ where $\mu_{N}$ is the set of $N$ th roots of unity. We can treat the weight 4 case similarly.

The result above in level 4 shows that the standard relations may be insufficient to determine $d(w, N)$. On the other hand, Deligne and Goncharov [4,5.25] provide some closed formulae for upper bounds of $d(w, N)$ for all $w$ and $N$ by studying the motivic fundamental group of $\mathbb{P}^{1}-\left(\{0, \infty\} \cup \boldsymbol{\mu}_{N}\right)$ in the framework of mixed Tate motives over the ring of $S$-integers of a number field. For example, one can deduce the bound $d(w, 4) \leqslant 2^{w}$ for all $w$. Further, Goncharov [5] defines some pro-nilpotent bi-graded Lie algebra $D$ using standard relations and then relates $D$ to the motivic fundamental Lie algebra in lower depth cases. Using this we shall improve the bounds of $d(w, N)$ in [4] for all levels $N=p$ and $N=p^{2}(p \geqslant 5$ a prime $)$.

To save space, throughout this note we will adopt the notation of [4] without further explanation.

## 2. Incompleteness of standard relations in $\mathcal{M P \mathcal { V }}(\boldsymbol{w}, 4)$

Fix $N=4$ throughout this section. In what follows we shall describe a process suggested by Deligne to verify that the standard relations cannot produce all possible $\mathbb{Q}$-linear relations in $\mathcal{M P \mathcal { V }}(w, 4)$.

Observe that the vector space freely generated by basis vectors corresponding to regularized MPVs of weight 3 and level 4 is dual to the degree 3 part of the free associative algebra $\mathbb{Q}\left\langle\left\langle e_{0}, e_{\zeta}\right\rangle\right\rangle_{\zeta \in \mu_{4}}$. One expects that $\mathcal{M} \mathcal{P} \mathcal{V}(w, 4)_{w \geqslant 1}$ is a weighted polynomial algebra with $2,1,2$, and 3 generators in weight 1 to 4 . The reason is that $\iota\left(\operatorname{Lie} U_{\omega}\right)$ should be a Lie algebra freely generated by one element in each degree so that the dimension of degree $n$ part is given by $\frac{1}{n} \sum_{d \mid n} \mu(n / d) 2^{d}-\delta_{1, n}$ (see [2, Ch. II, §3 Thm. 2]).

If one takes the space $\mathcal{M} \mathcal{P}(3,4)$ modulo the products of MPVs in lower weights one should get a quotient space of dimension 2 and one knows its dimension $\leqslant 2$. However, one can only prove the bound 3 by the standard relations as follows. Consider the subspace generated by the following elements:
I. For each MPV of weight 1 and MPV of weight 2 , the linear combination of weight 3 MPVs expressing their shuffle product by Chen's iterated integrals. This gives $5 \times 25$ elements.
II. Same for the stuffle product (quasi-shuffle as called by Hoffman) corresponding to the coproduct $\Delta_{*}$ in [7]. Plainly, these elements are linear combination of weight 3 MPVs expressing their stuffle products by series expansions (1). This gives $4 \times 20$ elements.
III. Distribution relations in weight 3: expressing the coefficient of a "convergent" monomial in $e_{0}$ and $e_{\alpha}(\alpha= \pm 1)$ as a multiple of the sum of the coefficients of the monomials deduced from it by replacing $e_{\alpha}$ by $e_{\beta}$ with $\beta^{2}=\alpha$. There are 12 "convergent" monomials to consider: ( $e_{0}$ or $e_{-1}$ ) ( $e_{0}$ or $e_{1}$ or $\left.e_{-1}\right)\left(e_{1}\right.$ or $\left.e_{-1}\right)$.
IV. Six regularized distribution relations in weight 3 (in [7, Prop. 2.26], change $\sigma^{n / d}=1$ to $\sigma^{d}=1$ ).

Elements from I to IV can be put into a $223 \times 125$ matrix. By MAPLE one can verify its rank is only 122 . Moreover, it is not hard to find three $\mathbb{Q}$-linearly independent relations which produce three vectors in the degree 2 part of the Lie
algebra denoted by $\mathfrak{d m r d}_{0}$ in [7]. In weight 4 the same procedure produces eight vectors instead of three which means one needs five more relations besides the standard ones.

## 3. Non-standard relations from octahedral symmetry of $\mathbb{P}^{\mathbf{1}}-\left(\{0, \infty\} \cup \mu_{4}\right)$

The punctured Riemann sphere $\mathbb{P}^{1}-\left(\{0, \infty\} \cup \mu_{4}\right)$ clearly possesses an octahedral symmetry. To use it one can adopt a system of tangent vectors stable (up to multiplication by $\boldsymbol{\mu}_{4}$ ) by the octahedral group. Hence one may take the tangential base points $1_{0}$ and (-2) (see [3]) and define the $\mathbb{C}$-linear map $\rho: \mathbb{Q}\left\langle\left\langle e_{0}, e_{\zeta}\right\rangle_{\zeta \in \mu_{4}} \rightarrow \mathbb{Q}\left\langle\left\langle e_{0}, e_{\zeta}\right\rangle_{\zeta \in \boldsymbol{\mu}_{4}}\right.\right.$ by

$$
\rho: e_{0} \rightarrow e_{1} \rightarrow e_{i} \rightarrow e_{0}, \quad e_{\infty} \rightarrow e_{-1} \rightarrow e_{-i} \rightarrow e_{\infty}
$$



Let $0<\varepsilon<1 / 3$ and $C_{\varepsilon}$ be the path $A_{1} \ldots A_{6}$ in the complex plane shown in the above picture, where $A_{2}, A_{4}$ and $A_{6}$ are the quarter circles of radii $\varepsilon, 2 \varepsilon$ and $2 \varepsilon$, respectively, oriented clockwise. Then by the property of iterated integrals

$$
\begin{equation*}
1=\int_{C_{\varepsilon}} \sum_{n=0}^{\infty} \Omega^{\circ n}=\int_{A_{6}} \sum_{n=0}^{\infty} \Omega^{\circ n} \int_{A_{5}} \sum_{n=0}^{\infty} \Omega^{\circ n} \cdots \int_{A_{1}} \sum_{n=0}^{\infty} \Omega^{\circ n}, \quad \text { where } \Omega=\sum_{a \in \mu_{4} \cup\{0\}} \frac{d z}{z-\sigma(a)} e_{a} . \tag{3}
\end{equation*}
$$

Replacing the straight path $1_{0} \rightarrow(-1)_{1}$ by the straight path $1_{0} \rightarrow(-2)_{1}$ changes dch $(\sigma)$ to

$$
\operatorname{dch}^{\prime}(\sigma)=\exp \left((\log 2) e_{1}\right) \operatorname{dch}(\sigma)
$$

(see $[4,5.16]$ for definition of $\operatorname{dch}(\sigma)$ ). So regularized integral over the path $A_{1}$ followed by $A_{2}$ gives $I=$ $\exp \left(-2 \pi i e_{1} / 4\right) \operatorname{dch}^{\prime}(\sigma)$. Thus (3) yields $\rho^{2}(I) \rho(I) I=1$, i.e.,

$$
\begin{equation*}
\exp \left(-2 L i_{1}(i) e_{0}\right) \rho^{2}(\operatorname{dch}(\sigma)) \exp \left(-2 L i_{1}(i) e_{i}\right) \rho(\operatorname{dch}(\sigma)) \exp \left(-2 L i_{1}(i) e_{1}\right) \operatorname{dch}(\sigma)=1 \tag{4}
\end{equation*}
$$

By comparing the coefficient of $e_{2} e_{1}^{2}$ in (4) and using Fact (*) one finally arrives at (2).
From [8, Table 2] one sees that $d(4,4) \leqslant 21$ by the standard relations. The five missing relations can now be found by comparing the coefficients of $e_{-i} e_{0}^{2} e_{-i}, e_{-i} e_{0}^{2} e_{-1}, e_{-i} e_{0}^{2} e_{i}, e_{-i} e_{0}^{2} e_{1}$, and ( $\left.e_{-i} e_{0}\right)^{2}$ in (4).

## 4. Weight two and level $\boldsymbol{p}$ or $\boldsymbol{p}^{\mathbf{2}}$ cases ( $\boldsymbol{p} \geqslant 5$ a prime)

Let $\mathcal{G}=\iota\left(\operatorname{Lie} U_{\omega}\right)$ (see [4, (5.12.2)]). By Remark 6.13 of [4] one may safely replace $\mathcal{G}_{N}^{(\ell)}$ by $\mathcal{G}$ throughout [5]. In particular, Goncharov's results can now be used to study the structure of Galois Lie algebra $\mathcal{G}_{\bullet, \bullet}\left(\boldsymbol{\mu}_{N}\right)=$ $\sum_{w \geqslant 1, l \geqslant 1} \mathcal{G}_{-w,-l}\left(\boldsymbol{\mu}_{N}\right)$ graded by the weight $w$ and depth $l$. Using these we obtain two results improving the bounds of $d(2, p)$ and $d\left(2, p^{2}\right)$ given in [4].

Theorem 1. Let $p \geqslant 5$ be a prime. Then $d(2, p) \leqslant(5 p+7)(p+1) / 24$. If Grothendieck's period conjecture [4,5.27(c)] is true then the equality holds and the standard relations in $\mathcal{M P V}(2, p)$ imply all the others.

Proof. One has $\operatorname{dim} \mathcal{G}_{-2,-1}\left(\boldsymbol{\mu}_{p}\right)=\frac{p-1}{2}$ and $\operatorname{dim} \mathcal{G}_{-2,-2}\left(\boldsymbol{\mu}_{p}\right)=\frac{(p-1)(p-5)}{12}$ by [5, Thm. 2.1, Cor. 2.16]. Define

$$
\begin{equation*}
\beta_{N}: \bigwedge^{2} \mathcal{G}_{-2,-1}\left(\boldsymbol{\mu}_{N}\right) \longrightarrow \mathcal{G}_{-2}\left(\boldsymbol{\mu}_{N}\right), \quad a \wedge b \longmapsto\{a, b\} \tag{5}
\end{equation*}
$$

where $\{$,$\} is the Ihara's Lie bracket [4,(5.13 .6)]$. Then

$$
\begin{equation*}
\operatorname{dim}\left(\operatorname{ker} \beta_{p}\right)=\frac{1}{2} \frac{p-1}{2}\left(\frac{p-1}{2}-1\right)-\frac{(p-1)(p-5)}{12}=\frac{p^{2}-1}{24} . \tag{6}
\end{equation*}
$$

Let DMRD $_{0}$ (see [7, $\S 3.2$, Thm. I]) be the affine subgroup of $\Pi$ (see [4, 5.7]) defined by only those polynomial equations satisfied by the coefficients of $\operatorname{dch}(\sigma)$ which are deduced from the standard relations, plus " $2 \pi i=0$ ", as explained in [4, 5.22]. Its Lie algebra $\mathfrak{d m r d}_{0}$ is graded by weight and depth, independent of the embedding by [7, Prop. 4.1] and contains $\mathcal{G}$ by [4, 5.22]. Further, Goncharov shows [5, §7.7] that the standard relations provide a complete list of constraints on the diagonal part of the Lie algebra $\mathcal{G}$ in depth $\leqslant 2$, yielding $\left(\mathfrak{d m r d}_{0}\right)_{m, m}=\mathcal{G}_{m, m}$ for $m=-1,-2$. Together with (6) this means in the proof of $[4,5.25]$ one can decrease the bound $D(2, p)$ by $\left(p^{2}-1\right) / 24$ and arrive at the bound $(5 p+7)(p+1) / 24$.

Grothendieck's conjecture implies that $\mathcal{G}=$ Lie $R$ where $R$ is the affine subgroup of $\Pi$ defined by all the polynomial equations satisfied by the coefficients of $\operatorname{dch}(\sigma)$ plus " $2 \pi i=0$ ". Thus one gets the equality in the theorem and the completeness of the standard relations. This concludes the proof of the theorem.

Now let $N=p^{2}$. By producing some nontrivial element in $\operatorname{ker} \beta_{p^{2}}$ we can show that
Theorem 2. If $p$ is a prime $\geqslant 5$ then $\operatorname{ker} \beta_{p^{2}} \neq 0$ and $d\left(2, p^{2}\right)<p^{2}(p-1)^{2} / 4$.
In fact, we find that $\operatorname{dim}\left(\operatorname{ker} \beta_{25}\right)=5$ and $\operatorname{dim}\left(\operatorname{ker} \beta_{49}\right)=35$ which implies $d(2,25) \leqslant 116$ and $d(2,49) \leqslant 449$ (see [8] for details). Further, if Grothendieck's conjecture holds then equalities follow. With MAPLE one can prove that $d(2,25) \leqslant 116$ and $d(2,49) \leqslant 449$ by using the standard relations so presumably these relations imply all the others. Finally, in all the other composite levels ( $7<N<50$ ) of weight 2, namely when $N$ is a 2 - or 3-power, or $N$ has at least two prime factors the standard relations are incomplete (see [8, Table 1]).

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