Standard Relations of Multiple Polylogarithm Values at Roots of Unity

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Abstract. Let \( N \) be a positive integer. In this paper we shall study the special values of multiple polylogarithms at \( N \)th roots of unity, called multiple polylogarithm values (MPVs) of level \( N \). These objects are generalizations of multiple zeta values and alternating Euler sums, which was studied by Euler, and more recently, many mathematicians and theoretical physicists. Our primary goal in this paper is to investigate the relations among the MPVs of the same weight and level by using the regularized double shuffle relations, regularized distribution relations, lifted versions of such relations from lower weights, and seeded relations which are produced by relations of weight one MPVs. We call relations from the above four families standard. Let \( d(w, N) \) be the \( \mathbb{Q} \)-dimension of \( \mathbb{Q} \)-span of all MPVs of weight \( w \) and level \( N \). Then we obtain upper bound for \( d(w, N) \) by the standard relations which in general are no worse or no better than the one given by Deligne and Goncharov depending on whether \( N \) is a prime-power or not, respectively, except for 2- and 3-powers, in which case standard relations seem to be often incomplete whereas Deligne shows that their bound should be sharp by a variant of Grothendieck’s period conjecture. This suggests that in general there should be other linear relations among MPVs besides the standard relations, some of which are written down in this paper explicitly with good numerical verification. We also provide a few conjectures which are supported by our computational evidence.

1 Introduction

In recent years, there is a revival of interest in multi-valued classical polylogarithms (polylogs) and their generalizations. For any positive integers \( s_1, \ldots, s_\ell \), Goncharov \cite{13} defines the multiple polylogs of complex variables as follows:

\[
Li_{s_1, \ldots, s_\ell}(x_1, \ldots, x_\ell) = \sum_{k_1 > \cdots > k_\ell > 0} \frac{x_1^{k_1} \cdots x_\ell^{k_\ell}}{k_1^{s_1} \cdots k_\ell^{s_\ell}}.
\]  

(1.1)

Conventionally one calls \( \ell \) the depth (or length) and \( s_1 + \cdots + s_\ell \) the weight. When the depth \( \ell = 1 \) the function is nothing but the classical polylog. When the weight is also 1 we get the MacLaurin series of \( -\log(1-x) \). Another useful expression of the multiple polylogs is given by the following iterated integral:

\[
Li_{s_1, \ldots, s_\ell}(x_1, \ldots, x_\ell) = (-1)^\ell \int_0^1 \left( \frac{dt}{t} \right)^{\alpha(s_1-1)} \circ \frac{dt}{t-a_1} \circ \cdots \circ \left( \frac{dt}{t} \right)^{\alpha(s_\ell-1)} \circ \frac{dt}{t-a_\ell}
\]  

(1.2)

where \( a_i = 1/(x_1 \cdots x_i) \) for \( 1 \leq i \leq \ell \). Here, we define the iterated integrals recursively by \( \int_a^b f(t) \circ w(t) = \int_a^b (\int_a^t f(t'))w(t) \) for any 1-form \( w(t) \) and concatenation of 1-forms \( f(t) \). We may think the path lies in \( \mathbb{C} \); however, it is more revealing to use iterated integrals in \( \mathbb{C}^\ell \) to find the analytic continuation of this function (see \cite{23}).
It is well-known that special values of polylogs have significant applications in arithmetic such as Zagier’s conjecture [23, p.622]. On the other hand, the multiple zeta values (MZV) appear naturally in the study of the fundamental group of $\mathbb{P}^1 - \{0, 1, \infty\}$ which is closely related to the absolute Galois group $\text{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ according the Grothendieck [9]. As pointed out by Goncharov, higher cyclotomy theory should study the multiple polylogs at roots of unity, not only those of the classical ones. Moreover, theoretical physicists have already found out that such values appear naturally in the study of Feynman diagrams ([5, 6]).

Starting from early 1990s Hoffman [15, 16] has constructed some quasi-shuffle (we will call “stuffle”) algebras reflecting the essential combinatorial properties of MZVs. Recently he [17] extends this to incorporate the multiple polylog values (MPVs) at roots of unity, although his definition of *-product is different from ours. Our approach here is a quantitative comparison between the the results obtained by Racinet [20] who considers MPVs from the motivic viewpoint of Drinfeld associators, and those by Deligne and Goncharov [11] who study the motivic fundamental groups of $\mathbb{P}^1 - \{(0, \infty) \cup \mu_N\}$ by using the theory of mixed Tate motives over S-integers of number fields, where $\mu_N$ is the group of Nth root of unity.

Fix an Nth root of unity $\mu = \mu_N := \exp(2\pi \sqrt{-1}/N)$. The level N MPVs are defined by

$$L_N(s_1, \ldots, s_l|v_1, \ldots, v_r) := L_{s_1, \ldots, s_l}(\mu^{v_1}, \ldots, \mu^{v_r}).$$

(1.3)

We will always identify $(i_1, \ldots, i_r)$ with $(i_1, \ldots, i_r) \pmod{N}$. It is easy to see from (1.1) that a MPV converges if and only if $(s_1, \mu^{v_1}) \neq (1, 1)$. Clearly, all level N MPVs are automatically of level $Nk$ for any positive integer k. For example when $i_1 = \cdots = i_r = 0$ or $N = 1$ we get the multiple zeta values $\zeta(s_1, \ldots, s_r)$. When $N = 2$ we recover the alternating Euler sums studied in [3, 25]. To save space, if a substring $S$ repeats $n$ times in the list then ${S}^n$ will be used. For example, $L_N({2}^2|{0}^2) = \zeta(2, 2) = \pi^4/120$.

Standard conjectures in arithmetic geometry imply that $\mathbb{Q}$-linear relations among MPVs can only exist between those of the same weight. Let $\mathcal{M}P(w, N)$ be the $\mathbb{Q}$-span of all the MPVs of weight $w$ and level $N$ whose dimension is denoted by $d(w, N)$. In general, to determine $d(w, N)$ precisely is a very difficult problem because any nontrivial lower bound would provide some nontrivial irrational/transcendental results which is related to a variant of Grothendieck’s period conjecture (see [10]). For example, we can easily show that $\mathcal{M}P(2, 4) = (\log^2 2, \pi^2, \pi \log 2\sqrt{-1}, (K - 1)\sqrt{-1})$, where $K = \sum_{n\geq 0}(-1)^n/(2n + 1)^2$ is the Catalan’s constant. From Grothendieck’s conjecture we know $d(2, 4) = 4$ (see op. cit.) but we don’t have a unconditional proof yet. On the other hand, we may obtain upper bound of $d(w, N)$ by finding as many linear relations in $\mathcal{M}P(w, N)$ as possible. As in the cases of MZVs and the alternating Euler sums the regularized double shuffle relations (RDS) play important roles in revealing the relations among MPVs. We shall study this theory for MPVs in section 4 by generalizing some results of [13] (also cf. [2]). It is commonly believed that in levels one and two all linear relations among MPVs are consequences of RDS.

From the point of view of Lyndon words and quasi-symmetric functions Bigotte et al. [2] have studied MPVs (they call them colored MZVs) primarily by using double shuffle relations. However, when the level $N \geq 3$, these relations are not complete in general, as we shall see in this paper.

If the level $N > 3$ then by a theorem of Bass [11] there are many non-trivial linear relations (regarded as seeds) in $\mathcal{M}P(1, N)$ whose structure is clear to us. Multiplied by MPVs of weight $w - 1$ these relations can produce non-trivial linear relations among MPVs of weight $w$ which we call the seeded relations. Similar to these relations we may produce new relations by multiplying MPVs on RDS of lower weights. We call such relations lifted relations. We conjecture that when level $N = 3$ all linear relations among MPVs are consequences of the RDS and the lifted RDS with $d(w, 3) = 2^w$.

Among MPVs we know that there are the so-called finite distribution relations (FDT). Racinet [20] considers further the regularization of these relations by regarding MPVs as the coefficients of some group-like element in a suitably defined pro-Lie-algebra of motivic origin. Our computation
shows that the regularized distribution relations (RDT) do contribute to new relations not covered by RDS and FDT. But they are not enough yet to produce all the lifted RDS.

**Definition 1.1.** We call a $\mathbb{Q}$-linear relation between MPVs *standard* if it can be produced by combinations of the following four families of relations: regularized double shuffle relations (RDS), regularized distribution relations (RDT), seeded relations, and lifted relations from the above. Otherwise, it is called a *non-standard* relation.

The main goal of this paper is to provide some numerical evidence concerning the (in)completeness of the standard relations. Namely, these relations in general are not enough to cover all the $\mathbb{Q}$-linear relation between MPVs (see Remark 9.2 and Remark 9.1); however, when the level is a prime $\leq 47$ and weight $w = 2$ using a result of Goncharov we can show that the standard relations are complete under the assumption of Grothendieck’s period conjecture (see [23]). We further find that when weight $w = 2$ and $N = 25$ or $N = 49$, the standard relations are complete. However, when $N$ is a 2-power or 3-power or has at least two distinct prime factors, we know that the standard relations are often incomplete by comparing our results with those of Deligne and Goncharov [11]. Moreover, we don’t know how to obtain the non-standard relations except that when $N = 4$, we discover recently that octahedral symmetry of $\mathbb{P}^1 - (\{0, \infty\} \cup \mu_4)$ can produce some (presumably all) new relations not covered by the standard ones (see op. cit.)

Most of the MPV identities in this paper are discovered with the help of MAPLE using symbolic computations. We have verified almost all relations by GiNaC [21] with an error bound $< 10^{-90}$.

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### 2 The double shuffle relations and the algebra $\mathfrak{A}$

It is Kontsevich [19] who first noticed that MZVs can be represented by iterated integrals (cf. [20]). We now extend this to MPVs. Set

$$a = \frac{dt}{t}, \quad b_i = \frac{\mu^i dt}{1 - \mu^i t} \quad \text{for } i = 0, 1, \ldots, N - 1.$$

For every positive integer $n$ define

$$y_{n,i} := a^{n-1}b_i.$$

Then it is straight-forward to verify using (1.2) that if $(s_1, \mu^{i_1}) \neq (1, 1)$ then (cf. [20] (2.5))

$$L_N(s_1, \ldots, s_n | i_1, i_2, \ldots, i_n) = \int_0^1 y_{s_1, i_1} y_{s_2, i_1 + i_2} \cdots y_{s_n, i_1 + i_2 + \cdots + i_n}.$$

We now define an algebra of words as follows:

**Definition 2.1.** Set $A_0 = \{1\}$ to be the set of the empty word. Define $\mathfrak{A} = \mathbb{Q}\langle A \rangle$ to be the graded noncommutative polynomial $\mathbb{Q}$-algebra generated by letters $a$ and $b_i$ for $i \equiv 0, \ldots, N - 1 \pmod{N}$, where $A$ is a locally finite set of generators whose degree $n$ part $A_n$ consists of words (i.e., a monomial in the letters) of depth $n$. Let $\mathfrak{A}^0$ be the subalgebra of $\mathfrak{A}$ generated by words not beginning with $b_0$ and not ending with $a$. The words in $\mathfrak{A}^0$ are called *admissible words*. 
Observe that every MPV can be expressed uniquely as an iterated integral over the closed interval \([0, 1]\) of an admissible word \(w\) in \(\mathcal{A}^0\). Then we denote this MPV by

\[
Z(w) := \int_0^1 w.
\]  

(2.2)

Therefore we have (cf. [20] (2.5) and (2.6))

\[
L_N(s_1, \ldots, s_n| i_1, i_2, \ldots, i_n) = Z(y_{s_1, i_1} y_{s_2, i_2} \cdots y_{s_n, i_n}),
\]

(2.3)

\[
Z(y_{s_1, i_1} y_{s_2, i_2} \cdots y_{s_n, i_n}) = L_N(s_1, \ldots, s_n| i_1, i_2 = i_1, \ldots, i_n = i_{n-1}).
\]

(2.4)

For example \(L_3(1, 2, 2|1, 0, 2) = Z(y_{1,1} y_{2,1} y_{2,2})\). On the other hand, during 1960s Chen developed a theory of iterated integral which can be applied in our situation.

**Lemma 2.2.** ([21] (1.5.1)) Let \(\omega_i\) \((i \geq 1)\) be \(\mathbb{C}\)-valued 1-forms on a manifold \(M\). For every path \(p\),

\[
\int_p \omega_1 \cdots \omega_r \int_p \omega_{r+1} \cdots \omega_{r+s} = \int_p (\omega_1 \cdots \omega_r) \mathfrak{m}(\omega_{r+1} \cdots \omega_{r+s})
\]

where \(\mathfrak{m}\) is the shuffle product defined by

\[
(\omega_1 \cdots \omega_r) \mathfrak{m}(\omega_{r+1} \cdots \omega_{r+s}) := \sum_{\sigma \in S_{r+s}, \sigma^{-1}(1) < \cdots < \sigma^{-1}(r)} \omega_{\sigma(1)} \cdots \omega_{\sigma(r+s)}.
\]

For example, we have

\[
L_N(1, 1)L_N(2, 3|1, 2) = Z(y_{1,1})Z(y_{2,1} y_{3,3}) = Z(b_1 \mathfrak{m}(ab_1 a^2 b_3))
\]

\[
= Z(b_1 ab_1 a^2 b_3 + 2ab_1 a^2 b_3 + (ab_1)^2 ab_3 + ab_1 a^2 b_3 + ab_1 a^2 b_3)
\]

\[
= Z(y_{1,1} y_{2,1} y_{3,3} + 2y_{2,1} y_{1,1} y_{3,3} + y_{2,1} y_{2,3} + y_{2,1} y_{3,1} y_{1,3} + y_{2,1} y_{3,3} y_{1,1})
\]

\[
= L_N(1, 2, 3|1, 0, 2) + 2L_N(2, 1, 3|1, 0, 2) + L_N(2, 2, 2|1, 0, 2)
\]

\[
+ L_N(2, 3, 1|1, 0, 2) + L_N(2, 3, 1|1, 2, N - 2).
\]

Let \(\mathfrak{A}^0_{\mathfrak{m}}\) be the algebra of \(\mathfrak{A}\) together with the multiplication defined by shuffle product \(\mathfrak{m}\). Denote the subalgebra \(\mathfrak{A}^0\) by \(\mathfrak{A}^0_{\mathfrak{m}}\) when we consider the shuffle product. Then we can easily prove

**Proposition 2.3.** The map \(Z : \mathfrak{A}^0_{\mathfrak{m}} \longrightarrow \mathbb{C}\) is an algebra homomorphism.

On the other hand, it is well known that MPVs also satisfy the series shuffle relations. For example

\[
L_N(2|5)L_N(3|4) = L_N(2, 3|5, 4) + L_N(3, 2|4, 5) + L_N(5|9).
\]

because

\[
\sum_{j > 0} \sum_{k > 0} = \sum_{j > k > 0} + \sum_{k > j > 0} + \sum_{j = k > 0}.
\]

To study such relations in general we need the following definition.

**Definition 2.4.** Denote by \(\mathfrak{A}^1\) the subalgebra of \(\mathfrak{A}\) which is generated by words \(y_{s, i}\) with \(s \in \mathbb{Z}_{>0}\) and \(i \equiv 0, \ldots, N - 1\) (mod \(N\)). Equivalently, \(\mathfrak{A}^1\) is the subalgebra of \(\mathfrak{A}\) generated by words not ending with \(a\). For any word \(w = y_{s_1, i_1} y_{s_2, i_2} \cdots y_{s_n, i_n} \in \mathfrak{A}^1\) and positive integer \(j\) we define the exponent shifting operator \(\tau_j\) by

\[
\tau_j(w) = y_{s_1, j+i_1} y_{s_2, j+i_2} \cdots y_{s_n, j+i_n}.
\]
For convenience, on the empty word we have the convention that \( \tau_{j}(1) = 1 \). We then define a new multiplication \(*\) on \( \mathfrak{A}^{1} \) by requiring that \(*\) distribute over addition, that \( 1 * w = w * 1 = w \) for any word \( w \), and that, for any words \( \omega_{1}, \omega_{2} \),

\[
y_{s,j}\omega_{1} * y_{t,k}\omega_{2} = y_{s,j}\left( \tau_{j}(\tau_{-j}(\omega_{1}) * y_{t,k}\omega_{2}) \right) + y_{t,k}\left( \tau_{k}(y_{s,j}\omega_{1} * \tau_{-k}(\omega_{2})) \right)
\]

\[
+ y_{s+t,i+j+k}\left( \tau_{j+k}(\tau_{-j}(\omega_{1}) * \tau_{-k}(\omega_{2})) \right). \tag{2.5}
\]

We call this multiplication the \textit{stuffle product}.

**Remark 2.5.** Our \( \mathfrak{A} \), \( \mathfrak{A}^{0} \) and \( \mathfrak{A}^{1} \) are related to \( \mathcal{Q}(X) \), \( \mathcal{Q}(X)_{cv} \) and \( \mathcal{Q}(Y) \) of [20], respectively. See section 5.

If we denote by \( \mathfrak{A}^{1}_{\ast} \) the algebra \((\mathfrak{A}^{1}, \ast)\), then it is not hard to show that (cf. [16, Thm. 2.1])

**Theorem 2.6.** The polynomial algebra \( \mathfrak{A}^{1}_{\ast} \) is a commutative graded \( \mathcal{Q} \)-algebra.

Now we can define the subalgebra \( \mathfrak{A}^{0}_{\ast} \) similar to \( \mathfrak{A}^{1}_{\ast} \) by replacing the shuffle product by stuffle product. Then by induction on the lengths and using the series definition we can quickly check that for any \( \omega_{1}, \omega_{2} \in \mathfrak{A}^{0} \)

\[
Z(\omega_{1})Z(\omega_{2}) = Z(\omega_{1} \ast \omega_{2}).
\]

This implies that

**Proposition 2.7.** The map \( Z : \mathfrak{A}^{0} \to \mathbb{C} \) is an algebra homomorphism.

For \( \omega_{1}, \omega_{2} \in \mathfrak{A}^{0} \) we will say that

\[
Z(\omega_{1} \ast \omega_{2} - \omega_{1} \ast \omega_{2}) = 0
\]

is a finite double shuffle (FDS) relation. It is known that even in level one these relations are not enough to provide all the relations among MZVs. However, it is believed that one can remedy this by considering RDS produced by the following mechanism. This was explained in detail in [18] when Ihara, Kaneko and Zagier considered MZVs where they call these extended double shuffle relations.

Combining Propositions 2.7 and 2.8 we can prove easily (cf. [18, Prop. 1]):

**Proposition 2.8.** We have two algebra homomorphisms:

\[
Z^{\ast} : (\mathfrak{A}^{1}_{\ast}, \ast) \to \mathbb{C}[T], \quad \text{and} \quad Z^{\mathfrak{I}} : (\mathfrak{A}^{1}_{\mathfrak{I}}, \mathfrak{I}) \to \mathbb{C}[T]
\]

which are uniquely determined by the properties that they both extend the evaluation map \( Z : \mathfrak{A}^{0} \to \mathbb{C} \) by sending \( b_{0} = y_{1,0} \) to \( T \).

In order to establish the crucial relation between \( Z^{\ast} \) and \( Z^{\mathfrak{I}} \) we can adopt the machinery in [18]. For any \( (s|t) = (s_{1}, \ldots, s_{N}|i_{1}, \ldots, i_{n}) \) where \( i_{j} \)'s are integers and \( s_{j} \)'s are positive integers, let the image of the corresponding words in \( \mathfrak{A}^{1} \) under \( Z^{\ast} \) and \( Z^{\mathfrak{I}} \) be denoted by \( Z^{\ast}_{(s|t)}(T) \) and \( Z^{\mathfrak{I}}_{(s|t)}(T) \) respectively. For example,

\[
T L_{N}(2|3) = Z^{\ast}_{(1|0)}(T)Z^{\ast}_{(2|3)}(T) = Z^{\ast}(y_{1,0} * y_{2,3})
\]

\[
= Z^{\ast}_{(1,2|0,3)}(T) + Z^{\ast}_{(2,1|3,3)}(T) + Z^{\ast}_{(3|3)}(T),
\]

while

\[
T L_{N}(2|3) = Z^{\mathfrak{I}}_{(1|0)}(T)Z^{\mathfrak{I}}_{(2|3)}(T) = Z^{\mathfrak{I}}(y_{1,0}y_{2,3}) = Z^{\mathfrak{I}}_{(0,0)}(T)
\]

\[
= Z^{\mathfrak{I}}_{(1,2|0,3)}(T) + Z^{\mathfrak{I}}_{(2,1|3,3)}(T) + Z^{\mathfrak{I}}_{(3|3)}(T).
\]

Hence we find the following RDS by the next Theorem:

\[
L_{N}(2, 1|3, 0) + L_{N}(3|3) = L_{N}(2, 1|3, N - 3) + L_{N}(2, 1|0, 3).
\]
Theorem 2.9. Define a $\mathbb{C}$-linear map $\rho : \mathbb{C}[T] \to \mathbb{C}[T]$ by
\[
\rho(e^{T u}) = \exp \left( \sum_{n=2}^{\infty} \frac{(-1)^n}{n} \zeta(n) u^n \right) e^{T u}, \quad |u| < 1.
\]
Then for any index set $(s|t)$ we have
\[
Z^R_{(s|t)}(T) = \rho(Z^*_{(s|t)}(T)).
\]
This is a the generalization of [18] Thm. 1 to the higher level MPV cases. The proof is essentially the same. One may compare Cor. 2.24 in [20]. The above steps can be easily transformed to computer codes which are used in our MAPLE programs.

3 Finite and regularized double shuffle relations (FDS & RDS)

It is generally believed that all the linear relations between MZVs can be derived from RDS. Although the naive generalization of this to arbitrary levels is wrong the idea in [18] to formalize this via some universal objects is still very useful. We want to generalize this idea to MPVs in this section.

Keep the same notation as in the preceding sections. Let $R$ be a commutative $\mathbb{Q}$-algebra with 1 and $Z_R : \mathbb{A}^0 \to R$ such that the "finite double shuffle" (FDS) property holds:
\[
Z_R(\omega_1 m \omega_2) = Z_R(\omega_1 * \omega_2) = Z_R(\omega_1) Z_R(\omega_2).
\]
We then extend $Z_R$ to $Z^R_R$ and $Z^*_R$ as before. Define an $R$-module $R$-linear automorphism $\rho_R$ of $R[T]$ by
\[
\rho_R(e^{T u}) = A_R(u)e^{T u}
\]
where
\[
A_R(u) = \exp \left( \sum_{n=2}^{\infty} \frac{(-1)^n}{n} Z_R(a^{n-1}b_0) u^n \right) \in R[[u]].
\]
Similar to the situation for MZVs, we may define the $\mathbb{A}^0$-algebra isomorphisms
\[
\text{reg}^T : \mathbb{A}^1_{\mathbb{M}} = \mathbb{A}^1_{\mathbb{M}}[b_0] \to \mathbb{A}^0_{\mathbb{M}}[T], \quad \text{reg}^*: \mathbb{A}^1_{*} = \mathbb{A}^0_{*}[b_0] \to \mathbb{A}^0_{*}[T],
\]
which send $b_0$ to $T$. Composing these with the evaluation map $T = 0$ we get the maps $\text{reg}^T_{\mathbb{M}}$ and $\text{reg}^*_{\mathbb{A}^1}$.

Theorem 3.1. Let $(R, Z_R)$ be as above with the FDS property. Then the following are equivalent:

(i) $(Z^R_R - \rho_R \circ Z^*_R)(w) = 0$ for all $w \in \mathbb{A}^1$.
(ii) $(Z^R_R - \rho_R \circ Z^*_R)(w)|_{T=0} = 0$ for all $w \in \mathbb{A}^1$.
(iii) $Z^R_R(\omega_1 m \omega_0 - \omega_1 * \omega_0) = 0$ for all $\omega_1 \in \mathbb{A}^1$ and all $\omega_0 \in \mathbb{A}^0$.
(iii') $Z^*_R(\omega_1 m \omega_0 - \omega_1 * \omega_0) = 0$ for all $\omega_1 \in \mathbb{A}^1$ and all $\omega_0 \in \mathbb{A}^0$.
(iv) $Z_R(\text{reg}^T_{\mathbb{M}}(\omega_1 m \omega_0 - \omega_1 * \omega_0)) = 0$ for all $\omega_1 \in \mathbb{A}^1$ and all $\omega_0 \in \mathbb{A}^0$.
(iv') $Z_R(\text{reg}^*_*(\omega_1 m \omega_0 - \omega_1 * \omega_0)) = 0$ for all $\omega_1 \in \mathbb{A}^1$ and all $\omega_0 \in \mathbb{A}^0$.
(v) $Z_R(\text{reg}^T_{\mathbb{M}}(b_0^m * w)) = 0$ for all $m \geq 1$ and all $w \in \mathbb{A}^0$. 

(\nu^\prime) \ Z_R(\text{reg}_s(b_0^s w - b_0^m w)) = 0 \ for \ all \ m \geq 1 \ and \ all \ w \in \mathbb{A}^0.

If \ Z_R \ satisfies \ any \ one \ of \ these \ then \ we \ say \ that \ Z_R \ has \ the \ regularized \ double \ shuffle \ (RDS) \ property.

Notice that RDS automatically implies FDS. The proof of the theorem is almost the same as that of [18 Thm. 2] but for completeness we give the most important details in the following because there is some subtle difference for MPVs of arbitrary level.

Denote by \( S \) the set of the \( y_{s,j} \) (\( s \in \mathbb{Z}_{\geq 0}, j = 0, \ldots, N - 1 \)). For convenience we write \( \tau_z = \tau_j \) if \( z = y_{s,j} \in S \). If \( w = y_{s_1,t_1} \ldots y_{s_n,t_n} \in \mathbb{A}^1 \) then we put \( \tau_w = \tau_{t_1+\ldots+t_n} \) and \( \tau_{-w} = \tau_{-t_1-\ldots-t_n} \). Then (cf. [18 Prop. 2])

**Proposition 3.2.** We have

(i) For \( z \in S \) the map \( \delta_z : \mathbb{A}^1 \rightarrow \mathbb{A}^1 \) defined by

\[
\delta_z(w) := z * w - z \tau_z(w)
\]

is a “twisted derivation” in the sense that

\[
\delta_z(w'w') = \delta_z(w)\tau_z(w') + w\tau_w(\delta_z(\tau_{-w}(w'))).
\]

Moreover, all these twisted derivations commute.

(ii) The above twisted derivations extend to a twisted derivation on all of \( \mathbb{A} \) after setting \( \tau_a = id \), with values on the letters \( a, b \) given by

\[
\delta_z(a) = 0, \quad \delta_z(b_j) = (a + b_j)\tau_j(z) \quad (z \in S, j = 0, \ldots, N - 1).
\]

In particular, \( \delta_z \) preserves \( \mathbb{A}^0 \).

**Proof.** Easy computation by Definition 2.5. \( \square \)

**Corollary 3.3.** Denote by \( \mathfrak{z} \) the \( \mathbb{Q} \)-linear span of the \( y_{s,0} \) \( (s \in \mathbb{Z}_{\geq 0}) \). Then for \( z \in \mathfrak{z} \) the map \( \delta_z \) is a derivation on \( \mathbb{A}^1 \) which preserves \( \mathbb{A}^0 \). Moreover, \( \delta_z \) can be extended to a derivation on \( \mathbb{A} \) by Prop. 3.2(ii).

**Proof.** Define \( \delta' \) as in Prop. 3.2(ii). For any \( z = y_{s,0} \in \mathfrak{z} \) and \( y_{t,i} \) a generator of \( \mathbb{A}^1 \) we have

\[
\delta'(y_{t,i}) = a^{t-1} \delta'(b_i) = a^{t-1}(a + b_i)y_{s,i} = y_{s,0} * y_{t,i} - y_{s,0}y_{t,i} = \delta_z(y_{t,i}).
\]

Note that for \( z \in \mathfrak{z} \) and \( w, w' \in \mathbb{A} \) we have \( \tau_w(\delta_z(\tau_{-w}(w'))) = \delta_z(w') \). So indeed \( \delta_z \) can be extended to a derivation on \( \mathbb{A} \). It’s obvious that \( \delta_z \) fixes both \( \mathbb{A}^0 \) and \( \mathbb{A}^1 \). \( \square \)

We can define another operation on \( S \) by \( y_{s,i} \circ y_{t,j} = y_{s+t,0+i+j} \). We can then restrict this to \( \{y_{s,0} : s \in \mathbb{Z}_{\geq 0}\} \) then extend linearly to \( \mathfrak{z} \). The following result is then straight-forward.

**Proposition 3.4.** The vector space \( \mathfrak{z} \) becomes a commutative and associative algebra with respect to the multiplication \( \circ \) defined by

\[
z \circ z' = z * z' - z z' - z' z.
\]

The following proposition is one of the keys to the proof of Theorem 3.1 (cf. [18 Prop. 4]).

**Proposition 3.5.** Let \( u \) be a formal variable. For \( z \in S \) we have

\[
\exp(zu\tau_z)(1) = (2 - \exp(zu\tau_z))^{-1}(1).
\]

(The inverse on the right is with respect to the concatenation product.)
Proposition 3.8. For all \( z \in \mathbb{S} \) we have

\[
\exp(z^2) = \exp(z) \circ z \exp(z)
\]

as desired.

Proof. Define power series

\[
f(uz) = \exp_o(zuz) - 1 = zu\tau_z + z \circ z \frac{u^2\tau_z^2}{2} + \cdots
\]

Then taking derivative with respect to \( u \) we get \( f'(uz) = z \circ (1 + f(uz))\tau_z \). Now for \( z, \omega \in \mathbb{S} \) we have by Prop. 3.2 and Prop. 3.5

\[
z * (\omega_1 \omega_2 \cdots \omega_n) = \sum_{i=0}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \omega_1 \cdots \omega_i \tau_{\omega_j}(z)\tau_z(\omega_{i+1} \cdots \omega_n) + \sum_{i=1}^{n} \omega_1 \cdots \omega_i \omega_{i-1}(z \circ \omega_i)\tau_z(\omega_{i+1} \cdots \omega_n).
\]

This yields

\[
z * \left(\prod_{i=1}^{n} (\frac{(uz)^{n_i}}{n_1!} \cdots \frac{(uz)^{n_d}}{n_d!})\right)
\]

\[
= \sum_{i=0}^{d} \left(\prod_{i=1}^{n} (\frac{(uz)^{n_i}}{n_1!} \cdots \frac{(uz)^{n_d}}{n_d!})\right) \tau_{\omega_i}(\frac{(uz)^{n_{i+1}}}{n_{i+1}!} \cdots \frac{(uz)^{n_d}}{n_d!})
\]

\[
+ \sum_{i=1}^{d} \left(\prod_{i=1}^{n} (\frac{(uz)^{n_i}}{n_1!} \cdots \frac{(uz)^{n_1}}{n_1!})\right) \tau_{\omega_i}(\frac{(uz)^{n_{i+1}}}{n_{i+1}!} \cdots \frac{(uz)^{n_d}}{n_d!}).
\]

Hence

\[
z * (1 - f(uz))^{-1} = \frac{d}{du} \left((1 - f(uz))^{-1}\right)(1).
\]

This implies that

\[
\exp(zuz)(1) = (1 - f(uz))^{-1}(1)
\]

as desired. \( \square \)

Corollary 3.6. For all \( z \in \mathbb{S} \) we have

\[
\exp(z\log_1(1 + z\tau)) = (1 - z\tau)^{-1}(1).
\]

If \( z \in \mathfrak{g} \) then \( \tau = \text{id} \) and therefore we have

Corollary 3.7. For \( z \in \mathfrak{g} \) we have

\[
\exp(zu) = (2 - \exp_o(zu))^{-1}, \quad \exp(z\log_1(1 + z)) = (1 - z)^{-1}.
\]

Let’s consider a non-trivial example of Cor. 3.6. Let \( N = 2 \) and \( z = y_{k,1} \) then we have

\[
\exp \left(\sum_{n=1}^{\infty} (-1)^{n-1} \zeta(nk; (-1)^{k}) \frac{u^n}{n}\right) = 1 + \sum_{n=1}^{\infty} \zeta({k}^n; {-1}^n) u^n
\]

where \( \zeta(s_1, \ldots, s_d; (-1)^{s_1}, \ldots, (-1)^{s_d}) = L_2(s_1, \ldots, s_d|\sigma_1, \ldots, \sigma_d) \) are the alternating Euler sums. For example, by comparing the coefficients of \( u^2 \) and \( u^3 \) we get \( 2\zeta(\overline{k}, \overline{k}) = \zeta(\overline{k})^2 - \zeta(2k) \), and \( 6\zeta(\overline{k}, \overline{k}, \overline{k}) = \zeta(\overline{k})^3 - 3\zeta(\overline{k})\zeta(2k) + 2\zeta(3k) \). Here \( \overline{k} \) means that the corresponding \( \sigma_j \) is odd.

The following two propositions are generalizations of Prop. 5-6 of [18] respectively whose computational proofs are mostly omitted since nothing new happens in our situation.

Proposition 3.8. For \( z, \zeta' \in \mathfrak{g} \) and \( w \in \mathfrak{A}_1 \) we have

\[
\exp(\delta_z)(z') = (\exp_o(z) \circ z') \exp_o(z), \quad \exp(\delta_z)(w) = (\exp_o(z))^{-1}(\exp_o(z) \circ w).
\]
Proposition 3.9. For $z \in \mathcal{J}$ define $\Phi_z : \mathfrak{A}^1 \rightarrow \mathfrak{A}^1$ by

$$\Phi_z(w) := (1 - z) \left( (1 - z)^{-1} \ast w \right) \quad (w \in \mathfrak{A}^1).$$

(3.3)

Then $\Phi_z$ is an automorphism of $\mathfrak{A}^1$ and we have

$$\Phi_z(w) = \exp(\delta_t)(w), \quad \text{where} \quad t = \log_2(1 + z) \in \mathcal{J}.$$  

(3.4)

All the $\Phi_z$ commute. Moreover, after restricting the derivation $\delta_t$ to $\mathfrak{A}^0$ we can regard $\Phi_z$ as an automorphism of $\mathfrak{A}^0$. If we extend the derivation $\delta_t$ to the whole $\mathfrak{A}$ as in Cor. 3.3 then we can regard $\Phi_z$ as an automorphism of $\mathfrak{A}$.

Proof. The key point is that $\delta_t$ sends $\mathfrak{A}^0$ to $\mathfrak{A}^0$ as a derivation by Cor. 3.3. Hence $\exp(\delta_t)$ is an automorphism on $\mathfrak{A}^1$ as well as on $\mathfrak{A}^0$.

The next three results are generalizations of Prop. 7, its corollary, and Prop. 8 of [18], respectively. The proofs there can be easily adapted into our situation because the $\mathfrak{m}$-product is essentially the same (note that the only essentially new phenomenon in the higher level MPV cases is that there are exponent shiftings on the roots of unity in our stuffle product.)

Proposition 3.10. Define the map $d : \mathfrak{A} \rightarrow \mathfrak{A}$ by $d(w) = b_0 \mathfrak{m} w - b_0 w$. Then $d$ is a derivation and by setting $u$ as a formal parameter we have

$$\exp(du)(w) = (1 - b_0 u)^{-1} \left( (1 - b_0 u)^{-1} \mathfrak{m} w \right) \quad (w \in \mathfrak{A}^1).$$

(3.5)

On the generators we have

$$\exp(du)(a) = a(1 - b_0 u)^{-1}, \quad \exp(du)(b_j) = b_j (1 - b_0 u)^{-1}, \quad j = 0, \ldots, N - 1.$$  

(3.5)

Remark 3.11. In fact, we can replace the whole $\mathfrak{A}$ by $\mathfrak{A}^1$ in the first part of Prop. 3.10. We can do the same in the next corollary. However, in the proof of Theorem 3.1 we only need this weaker version.

Corollary 3.12. Let $u$ be a formal parameter. Let $\Delta_u = \exp(-du) \circ \Phi_{b_0 u} \in \text{Aut}(\mathfrak{A}) [u]$ (here $\circ$ means the composition). Then

$$(1 - b_0 u)^{-1} \ast w = (1 - b_0 u)^{-1} \mathfrak{m} \Delta_u(w), \quad \forall w \in \mathfrak{A}^1.$$  

In particular, for $w \in \mathfrak{A}^0$ by taking reg on both sides of the above equation we get

$$\text{reg} \left( (1 - b_0 u)^{-1} \ast w \right) = \Delta_u(w).$$

Proposition 3.13. For $\omega_0 = a \omega'_0 \in \mathfrak{A}^0$ we have

$$\text{reg}^T \left( (1 - b_0 u)^{-1} \ast \omega_0 \right) = \exp(-du)(\omega_0)e^{Tu} = a \left( (1 + b_0 u)^{-1} \mathfrak{m} \omega'_0 \right) e^{Tu}.$$  

Remark 3.14. Theorem 3.1 now follows easily from a detailed computation as in [18]. As a matter of fact, the same argument shows that [18, Prop. 10] and its Cor. are both valid in our general setup if we replace $\mathcal{J}^0$ there by $\mathfrak{A}^0$.

4 Seeded (or weight one) relations

When $N \geq 4$ there exist linear relations among MPVs of weight one by a theorem of Bass [1]. These relations are important because by multiplying any MPV of weight $w - 1$ by such a relation
Multiple polylogs satisfy the following distribution formula (cf. \[20, Prop. 2.25\]):

\[
\text{Regularized distribution relations for all positive integer } d
\]

\[\text{or every path } Q\]

\[\text{Then one may consider the coproduct } \Delta \text{ of forms in words: for all }\]

\[\text{symmetric relation } (FDT).\]

Racinet further considers the regularized version of these relations, \(L\),

\[\text{Hence there are many linear relations among } L_N(1|j).\]

For instance, if \(j < N/2\) then we have the symmetric relation

\[- \log(1 - \mu^j) = - \log(1 - \mu^{N-j}) - \log(-\mu^j) = - \log(1 - \mu^{N-j}) + \frac{N - 2j}{N} \pi \sqrt{-1}.\]

Thus for all \(1 < j < N/2\)

\[(N - 2)(L_N(1|j) - L_N(1|N - j)) = (N - 2j)(L_N(1|1) - L_N(1|N - 1)).\]  \(4.1\)

Further, from \([1, (B)]\) for any divisor \(d\) of \(N\) and \(1 \leq a < d' := N/d\) we have the distribution relation

\[
\sum_{0 \leq j < d} L_N(1|a + jd') = L_N(1|ad).\]  \(4.2\)

It follows from the main result of Bass \([1]\) corrected by Ennola \([2]\) that all the linear relations between \(L_N(1|j)\) are consequences of \((4.1)\) and \((4.2)\). Hence the seeded relations have the following forms in words: for all \(w \in \mathfrak{A}^0\)

\[
\begin{cases}
(N - 2)Z(y_{1,j} * w - y_{1,-j} * w) = (N - 2j)(Z(y_{1,1} * w - y_{1,-1} * w), \\
\sum_{0 \leq j < d} Z(y_{1,a + jd'} * w) = Z(y_{1,ad} * w).
\end{cases}
\]  \(4.3\)

5 Regularized distribution relations

Multiple polylogs satisfy the following distribution formula (cf. \[20, Prop. 2.25\]):

\[
L_{s_1, \ldots, s_n}(x_1, \ldots, x_n) = \left| \begin{array}{c}
\end{array} \right| + \cdots + s_n - n
\]

\[
\sum_{y^j = x, 1 \leq j \leq n} L_{s_1, \ldots, s_n}(y_1, \ldots, y_n),\]  \(5.1\)

for all positive integer \(d\). When \(s_1 = 1\) we need to exclude the case of \(x_1 = 1\). We call these finite distribution relations \((FDT)\). Racinet further considers the regularized version of these relations, which we now recall briefly.

Fix an embedding \(\mu_N \rightarrow \mathbb{C}\) and denote by \(\Gamma\) its image. Define two sets of words

\[
\mathbf{X} := X_{\Gamma} = \{x_\sigma : \sigma \in \Gamma \cup \{0\}\}, \quad \text{and} \quad \mathbf{Y} := Y_{\Gamma} = \{y_{n,\sigma} = x_0^{n-1} x_\sigma : n \in \mathbb{N}, \sigma \in \Gamma\}.
\]

Then one may consider the coproduct \(\Delta\) of \(\mathbb{Q}\langle \mathbf{X} \rangle\) defined by \(\Delta x_\sigma = 1 \otimes x_\sigma + x_\sigma \otimes 1\) for all \(\sigma \in \Gamma \cup \{0\}\). For every path \(\gamma \in \mathbb{P}^1(\mathbb{C}) - ([0, \infty) \cup \Gamma)\) Racinet defines the group-like element \(I_\gamma \in \mathbb{C}[\langle \mathbf{X} \rangle]\) by

\[
I_\gamma := \sum_{\rho \in \mathbb{N}, \sigma_1, \ldots, \sigma_p \in \Gamma \cup \{0\}} I_\gamma(\sigma_1, \ldots, \sigma_p)x_{\sigma_1} \cdots x_{\sigma_p}.
\]
where \( I_\gamma(\sigma_1, \ldots, \sigma_p) \) is the iterated integral \( \int_\gamma \omega(\sigma_1) \cdots \omega(\sigma_p) \) with

\[
\omega(\sigma)(t) = \begin{cases} 
\sigma \frac{dt}{1 - \sigma t}, & \text{if } \sigma \neq 0; \\
\frac{dt}{t}, & \text{if } \sigma = 0.
\end{cases}
\]

This \( I_\gamma \) is essentially the same element denoted by \( \text{dch} \) in [11]. Note that \( \mathbb{Q} \langle Y \rangle \) is the sub-algebra of \( \mathbb{Q} \langle X \rangle \) generated by words not ending with \( x_0 \). We let \( \pi_Y : \mathbb{Q} \langle X \rangle \to \mathbb{Q} \langle Y \rangle \) be the projection. As \( x_0 \) is primitive one knows that \( (\mathbb{Q} \langle Y \rangle, \Delta) \) has a graded co-algebra structure.

Let \( \mathbb{Q} \langle X \rangle_{cv} \) be the sub-algebra of \( \mathbb{Q} \langle X \rangle \) not beginning with \( x_1 \) and not ending with \( x_0 \). Let \( \pi_{cv} : \mathbb{Q} \langle X \rangle \to \mathbb{Q} \langle X \rangle_{cv} \) be the projection. Passing to the limit one get:

**Proposition 5.1.** ([20 Prop.2.11]) The series \( I_{cv} := \lim_{a \to 0^+, b \to 1^-} \pi_{cv}(I_{[a,b]}) \) is group-like in \( (\mathbb{C} \langle X \rangle)_{cv}, \Delta) \).

Let \( I \) be the unique group-like element in \( (\mathbb{C} \langle X \rangle), \Delta) \) whose coefficients of \( x_0 \) and \( x_1 \) are 0 such that \( \pi_{cv}(I) = I_{cv} \). In order to do the numerical computation we need to find out explicitly the coefficients for \( I \). Put

\[
I = \sum_{p \in \mathbb{N}, \sigma_1, \ldots, \sigma_p \in \Gamma \cup \{0\}} C(\sigma_1, \ldots, \sigma_p)x_{\sigma_1} \cdots x_{\sigma_p}.
\]

**Proposition 5.2.** Let \( p, m \) and \( n \) be three non-negative integers. If \( p > 0 \) then we assume \( \sigma_1 \neq 1 \) and \( \sigma_p \neq 0 \). Set \( (\sigma_1, \ldots, \sigma_p, \{0\}^n) = (\sigma_1, \ldots, \sigma_q) \). Then we have

\[
C(\{1\}^m, \sigma_1, \ldots, \sigma_p, \{0\}^n) = \begin{cases} 
0, & \text{if } mn = p = 0; \\
Z(\pi_Y(x_{\sigma_1} \cdots x_{\sigma_p})), & \text{if } m = n = 0; \\
-\frac{1}{m} \sum_{i=1}^{q} C(\{1\}^{m-1}, \sigma_1, \ldots, \sigma_{i-1}, 1, \sigma_{i+1}, \ldots, \sigma_q), & \text{if } m > 0; \\
-\frac{1}{n} \sum_{i=1}^{p} C(\sigma_1, \ldots, \sigma_{i-1}, 0, \sigma_{i}, \ldots, \sigma_p, \{0\}^{n-1}), & \text{if } m = 0, n > 0.
\end{cases}
\]

(5.2)

Here \( Z \) is defined by (2.2).

**Remark 5.3.** This proposition provides the recursive relations we may use to compute all the coefficients of \( I \).

**Proof.** Since \( I \) is group-like we have

\[
\Delta I = I \otimes I.
\]

The first case follows from this immediately since \( C(0) = C(1) = 0 \). The second case is essentially the definition (2.2) of \( Z \). If \( m > 0 \) then we can compare the coefficient of \( x_1 \otimes x_1^{m-1}x_{\sigma_1} \cdots x_{\sigma_q} \) of the two sides of (5.3) and find the relation (5.2). Finally, if \( m = 0 \) and \( n > 0 \) then we may similarly consider the coefficient of \( x_{\sigma_1} \cdots x_{\sigma_p}x_0^{n-1} \otimes x_0 \) in (5.3). This finishes the proof of the proposition.

For any divisor \( d \) of \( N \) let \( \Gamma^d = \{ \sigma^d : \sigma \in \Gamma \} \), \( i_d : \Gamma^d \to \Gamma \) the embedding, and \( p^d : \Gamma \to \Gamma^d \) the \( d \)th power map. They induce two algebra homomorphisms:

\[
p^d_* : \mathbb{Q} \langle X \rangle \to \mathbb{Q} \langle X_{\Gamma^d} \rangle \] and \[i_d^* : \mathbb{Q} \langle X \rangle \to \mathbb{Q} \langle X_{\Gamma^d} \rangle \]

\[
x_\sigma \mapsto \begin{cases} 
 dx_0, & \text{if } \sigma = 0; \\
x_{\sigma^d}, & \text{if } \sigma \in \Gamma.
\end{cases}
\]

and

\[
x_\sigma \mapsto \begin{cases} 
 x_0, & \text{if } \sigma = 0, \\
x_\sigma, & \text{if } \sigma \in \Gamma^d, \\
0, & \text{otherwise.}
\end{cases}
\]
It is easy to see that both $i^d_\sigma$ and $p^d_\sigma$ are $\Delta$-coalgebra morphisms such that $i^d_\sigma(I)$ and $p^d_\sigma(I)$ have the same image under the map $\pi_\infty$. By the standard Lie-algebra mechanism one has

**Proposition 5.4.** ([20 Prop.2.26]) For every divisor $d$ of $N$

$$p^d_\sigma(I) = \exp \left( \sum_{\sigma \neq 1, \sigma \neq 1}^{\sigma^d = 1} L_i(\sigma)x_1 \right) i^d_\sigma(I).$$

(5.4)

Combined with Proposition [5.2] the above result provides the so-called regularized distribution relations (RDT) which of course include all the FDT of MPVs given by [5.1].

Computation suggests the following conjecture concerning a special class of distribution relations.

**Conjecture 5.5.** Let $d$ be a positive integer. Then all the distribution relations in [5.1], where $x_j = 1$ for all $j$, are consequences of RDS of MPVs of level $d$.

We are able to confirm this conjecture in the special case that $w = 2$, $n = 1$, and $d$ is a prime.

**Theorem 5.6.** Write $L(i, j) = L_p(1,1|i, j)$ and $D(i) = L_p(2|i)$. Define for $1 \leq i, j < p$:

$$\text{FDT} := D(0) - p \sum_{j=0}^{p-1} D(j) = 0, \quad \text{RDS}(i) := D(i) + L(i,0) - L(i, -i) = 0,$$

$$\text{FDS}(i, j) := D(i + j) + L(i, j) + L(j, i) - L(i, j - i) - L(j, i - j) = 0.$$

Then

$$\text{FDT} = \sum_{1 \leq i < p} \text{FDS}(i, i) + 2 \sum_{1 \leq j < i < p} \text{FDS}(i, j) + 2 \sum_{i=1}^{p-1} \text{RDS}(i, i).$$

(5.5)

**Proof.** By changing the order of summation we see that

$$2 \sum_{1 \leq j < i < p} D(i + j) = \sum_{i=2}^{p-1} \sum_{j=1}^{p-1} D(i + j) + \sum_{j=1}^{p-1} \sum_{i=2}^{p-1} D(i + j)$$

$$= \sum_{i=2}^{p-1} \sum_{j=1}^{p-1} D(i + j) + \sum_{j=1}^{p-1} D(j - 1) + \sum_{i=2}^{p-1} D(i + 1)$$

$$= (p - 3) \sum_{j=0}^{p-1} D(j) - \sum_{i=2}^{p-1} D(i) - \sum_{i=1}^{p-1} D(2i) + \sum_{j=1}^{p-2} D(j) + \sum_{j=2}^{p-1} D(j) + 2D(0)$$

$$= (p - 1)D(0) + (p - 3) \sum_{j=1}^{p-1} D(j)$$

since $\sum_{j=0}^{p-1} D(i + j) = \sum_{i=1}^{p-1} D(j)$ for all $i$ and $\sum_{i=1}^{p-1} D(2i) = \sum_{i=1}^{p-1} D(i)$. This implies that the dilogarithms on the right hand side of (5.5) exactly add up to FDT. Thus we only need to show that all the double logarithms on the right hand side of (5.5) cancel.

First we note that $L(0,0)$ in FDS$(i, i)$ and RDS$(i, i)$ cancel. Now let us consider the lattice points $(i, j)$ of $\mathbb{Z}^2$ corresponding to $L(i, j)$. The points $(i, j)$ corresponding to $L(i, j)$ with positive signs fill in exactly the area inside the square $[1, p - 1] \times [1, p - 1]$ (boundary inclusive): $L(i, j)$ in FDS$(i, i)$ provides the diagonal $y = x, \sum_{1 \leq j < i < p} L(i, j)$ (resp. $\sum_{1 \leq j < i < p} L(j, i)$) form the lower right (resp. upper left) triangular region.

For the negative terms of the double logs, $L(i, -i)$ in RDS$(i)$ provides the diagonal $x + y = p, \sum_{1 \leq j < i < p} L(i, j - i)$ of $L(i, j - i)$ form the upper right triangular region. Similarly, by changing the order of summation $\sum_{1 \leq j < i < p} L(j, i - j) = \sum_{i=1}^{p-2} \sum_{j=i+1}^{p-1} L(i, j - i) = \sum_{i=2}^{p-2} \sum_{j=1}^{p-1-i} L(i, j)$ fills the lower left region. \qed
Further, numerical evidence up to level $N = 49$ supports the following

**Conjecture 5.7.** In weight two, all RDT are consequences of RDS and FDT.

## 6 Lifted relations from lower weights

Note that when $N = 3$ there are no seeded relations nor (regularized) distribution relations. When we deal with MZVs and alternating Euler sums we expect that all the linear relations come from RDS. Are these enough when $N = 3$? Surprisingly, the answer is no.

The first counterexample is in weight four, i.e., $(w, N) = (4, 3)$. Easy computation shows that there are 144 MPVs in this case among which there are 239 nontrivial RDS which include 191 FDS. Using these relations we get 127 independent linear relations among the 144 MPVs. But the upper bound of $d(4, 3)$ by $[11, 5.25]$ is 16, so there must be at least one more linearly independent relation. Where else can we find it? It is easy to verify that all the seven RDT (including four FDT) can be derived from RDS. However, we know that a product of two weight two MPVs is of weight four. So on each of the five RDS (including two FDS) in $\mathcal{MPV}(2, 3)$ we can multiply any one of the nine MPVs of $(w, N) = (2, 3)$ to get a relation in $\mathcal{MPV}(4, 3)$. For instance, we have a FDS

$$Z(y_{1, 1} * y_{1, 1} - y_{1, 1} y_{1, 1}) = L_3(2|2|2) + 2L_3(1|1|1, 1) - L_3(1|1, 1|0) = 0.$$  

Multiplying by $L_3(1|1, 1|1) = Z(y_{1, 1} y_{1, 2})$ we have a new relation not derivable from RDS in $\mathcal{MPV}(4, 3)$:

$$Z(y_{1, 1} y_{1, 2} y_{2, 0} + 2y_{1, 1} y_{1, 2} - 2y_{1, 1} y_{1, 0})$$

$$= L_3(1, 1|2|1, 1, 0) + 2L_3(1, 2|1|1, 1, 0) + 2L_3(2, 1|1|1, 1, 0) + L_3(2, 1|1|2, 2, 1) + 4L_3(4|1, 1, 2, 1) + 8L_3(4|1, 0, 0, 1) - 6L_3(4|1, 1|1, 1, 1, 1) - 2L_3(4|1, 1, 1|1, 2, 0) = 0.$$  

Such relations coming from the lower weights are called *lifted relations (from lower weights).* In this way, when $(w, N) = (4, 3)$ we can produce 45 lifted RDS relations from weight two, 58 from weight three. We may also lift RDT and obtain nine and six relations from weight two and three, respectively. However, all the lifted relations together only produce one new linearly independent relation, as expected. Hence we find totally 128 linearly independent relations among the 144 MPVs of $(w, N) = (4, 3)$. This implies that $d(4, 3) \leq 16$ which is the same bound obtained by $[11, 5.25]$ and is proved to be exact under a variant of Grothendieck’s period conjecture by Deligne $[10]$.

For general levels $N$ we may lift not only RDS and RDT but also the seeded relations. But a moment reflection tells us that the lifted seeded relations are seeded so we don’t need to consider these after all.

**Definition 6.1.** We call a $\mathbb{Q}$-linear relation between MPVs *standard* if it can be produced by combinations of the following four families of relations: regularized double shuffle relations (RDS), regularized distribution relations (RDT), seeded relations, and lifted relations from the above. Otherwise, it is called a *non-standard* relation.

There are no seeded relations if $N = 3$. In this case we believe that all the linear relations among MPVs come from RDS and the lifted relations (see Conjecture $[7]$). Moreover, computation in small weight cases supports the following

**Conjecture 6.2.** Suppose $N = 3$ or 4. Every MPV of level $N$ is a linear combination of MPVs of the form $L((1)^w t_1, \ldots, t_w)$ with $t_j \in \{1, 2\}$. Consequently, the $\mathbb{Q}$-dimension of the MPVs of weight $w$ and level $N$ is given by $d(w, N) = 2^w$ for all $w \geq 1$.

**Remark 6.3.** Even adding all the lifted relations from lower weights does not provide all the linear relations among MPVs. A quick look at the Table $[2]$ in $[8]$ tells us that if $(w, N) = (3, 4)$ even though
we know $d(3, 4) \leq 8$ and $d(4, 4) \leq 16$ by [11] 5.25, and the equality should hold by Conjecture 6.2 or by a variant of Grothendieck’s period conjecture (see Remark 6.4), we cannot produce enough relations by using the standard ones. Instead, we can only show that $d(3, 4) \leq 9$ and $d(4, 4) \leq 21$. More recently, by using octahedral symmetry of $P$, we know $d(w, 3) = d(w, 4) = 2^w$, and $d(w, 8) = 3^w$.

7 Some conjectures of FDS and RDS

Recall that if a map $Z_R : \mathcal{A}^0 \to R$ satisfies the FDS and any one of the equivalent conditions in Theorem 6.1 then we say that $Z_R$ has the regularized double shuffle (RDS) property. Let $R_{RDS}$ be the universal algebra (together with a map $Z_{R_{RDS}} : \mathcal{A}^0 \to R_{RDS}$) such that for every $\mathcal{Q}$-algebra $R$ and a map $Z_R : \mathcal{A}^0 \to R$ satisfying RDS there always exists a map $\varphi_R$ to make the following diagram commutative:

\[
\begin{array}{ccc}
\mathcal{A}^0 & \xrightarrow{Z_{R_{RDS}}} & R_{RDS} \\
\xrightarrow{Z_R} & & \xleftarrow{\varphi_R} \\
R & \xrightarrow{\varphi_R} & \end{array}
\]

When $N = 3$ computation shows that the lifted relations contribute non-trivially when the weight $w = 5$: we can only get $d(5, 3) \leq 33$ instead of the conjecturally correct dimension 32 without using lifted relations. We may say that $Z_R$ has the lifted regularized double shuffle (LRDS) property if it satisfies RDS and for all $\omega_0, \omega_0', \omega_0'' \in \mathcal{A}^0$

\[
Z_R(Z_R^{-1} \circ \rho_R \circ Z_R(\omega_0) * \omega_0 - \omega_0 * \omega_0) = Z_R((\omega_0 * \omega_0') * \omega_0'' - (\omega_0 \mathbf{i} \omega_0') * \omega_0'') = 0.
\]

We can define $Z_{SR}$ and $R_{SR}$ corresponding to the standard relations similar to $Z_{RDS}$ and $R_{RDS}$ such that for every $\mathcal{Q}$-algebra $R$ and a map $Z_R : \mathcal{A}^0 \to R$ satisfying the standard relations there always exists a map $\varphi_R$ to make the following diagram commutative:

\[
\begin{array}{ccc}
\mathcal{A}^0 & \xrightarrow{Z_{SR}} & R_{SR} \\
\xrightarrow{Z_R} & & \xleftarrow{\varphi_R} \\
R & \xrightarrow{\varphi_R} & \end{array}
\]

Conjecture 7.1. Let $(R, Z_R) = (\mathbb{R}, Z)$ if $N = 1, 2$ and $(R, Z_R) = (\mathbb{C}, Z)$ if $N = p$ is a prime $\geq 3$, where $Z$ is given by 6.2. If $N = 1$ or 2 then the map $\varphi_R$ is injective, namely, the algebra of MPVs is isomorphic to $R_{RDS}$. If $N = p$ is a prime $\geq 3$ then the map $\varphi_R$ is injective so the algebra of MPVs of level $p$ is isomorphic to $R_{SR}$. Moreover, if $N = 3$ then $Z_{LRDS} = Z_{SR}$ and $R_{LRDS} = R_{SR}$.

From Conjecture 7.1 all the linear relations among MPVs can be produced by RDS when $N = 1$ or 2, and by the standard ones when $N = p$ is prime $\geq 3$. When $p \geq 5$ this is proved in [24] under the assumption of Grothendieck’s period conjecture.

Computation in many cases such as those listed in Remark 9.2 and 9.1 show that MPVs must satisfy some other relations besides the standard ones when $N$ has more than two distinct prime factors, so a naive generalization of Conjecture 7.1 to all levels does not exist at present. However, when $N = 4$ we find that octahedral symmetry of $\mathbb{P}^1 - \{0, \infty\} \cup \mu_4$ may provide all the non-standard relations (see [24]). But since we only have numerical evidence in weight 3 and 4 it may be a little premature to form a conjecture for level four at present.
8 The structure of MPVs and some examples

In this section we concentrate on RDS between MPVs of small weights. Most of the computations in this section are carried out by MAPLE. We have checked the consistency of these relations with many known ones and verified our results numerically using GiNaC [21] and EZ-face [4].

By considering all the admissible words we see easily that the number of distinct MPVs of weight \( w \geq 2 \) and level \( N \) is \( N^2(N+1)^w-2 \) and there are at most \( N(N+1)^w-2 \) RDS (but not FDS). If \( w \geq 4 \) then the number of FDS is given by
\[
(N-1)N^2(N+1)^w-3 + \left( \frac{w}{2} - 1 \right) N^4(N+1)^w-4 = \left( N^2 \left( \frac{w}{2} - 1 \right) N^2(N+1)^w-4. 
\]
If \( w = 2 \) (resp. \( w = 3 \)) then the number of FDS is \( (N-1)^2 \) (resp. \( N^2(N-1) \)).

8.1 Weight one.

From [41] we know that all relations in weight one follow from (4.1) and (4.2), and no RDS exists. The relations in weight one are crucial for higher level cases because they provide the seeded relations considered in [41]. Moreover, easy computation by (4.1) and (4.2) shows that there is a hidden integral structure, namely, in each level there exists a Q-basis consisting of MPVs such that every other MPV is a Z-linear combination of the basis elements. This fact is proved by Conrad [8, Theorem 4.6]. Similar results should hold for higher weight cases and we hope to return to this in a future publication [26].

8.2 Weight two.

There are \( N^2 \) MPVs of weight 2 and level \( N \):
\[
L_N(1,1|i,j), \quad L_N(2|j), \quad 1 \leq i \leq N-1, 0 \leq j \leq N-1.
\]
For \( 1 \leq i, j < N \) the FDS \( Z^*(y_{1,i} \ast y_{1,j}) = Z^{\text{III}}(y_{1,i} \ast y_{1,j}) \) yields
\[
L_N(2|i+j) + L_N(1,1|i,j) + L_N(1,1|j,i) = L_N(1,1|i,j-i) + L_N(1,1|j,i-j). \tag{8.1}
\]
Now from RDS \( \rho(Z^*(y_{1,0} \ast y_{1,i})) = Z^{\text{III}}(y_{1,0} \ast y_{1,i}) \) we get for \( 1 \leq i < N \)
\[
L_N(1,1|i,0) + L_N(2|i) = L_N(1,1|i,-i). \tag{8.2}
\]
The FDT in (5.1) yields: for every divisor \( d \) of \( N \), and \( 1 \leq a, b < d' := N/d \)
\[
L_N(2|ad) = \sum_{j=0}^{d-1} L_N(2|a+jd'), \tag{8.3}
\]
\[
L_N(1,1|ad,bd) = \sum_{j,k=0}^{d-1} L_N(1,1|a+jd',b+kd'). \tag{8.4}
\]
To derive the RDT we can compare the coefficients of \( x_1 x_{\mu d} \) in (5.4) and use Prop. 5.2 to get: for every divisor \( d \) of \( N \), and \( 1 \leq a < d' \)
\[
L_N(1|ad)\sum_{j=1}^{d-1} L_N(1|jd') = \sum_{j=1}^{d-1} \sum_{k=0}^{d-1} L_N(1,1|jd',a+kd')
- \sum_{k=0}^{d-1} L_N(1,1|a+kd',-a-kd') - L_N(1,1|ad,-ad). \tag{8.5}
\]
By definition, the seeded relations are obtained from \(4.1\) and \(4.2\). For example, if \(N = p\) is a prime then \(4.2\) is trivial and \(4.1\) is equivalent to: for all \(1 \leq j < h := (p - 1)/2\)

\[
L_N(1|j) - L_N(1|j) = (p - 2j)(L_N(1|h) - L_N(1|h + 1)).
\] (8.6)

Thus multiplying by \(L_N(1|i)\) \((1 \leq i < p)\) and applying the shuffle relation \(L_N(1|a)L_N(1|b) = L_N(1,1|a,b - a) + L_N(1,1|b,a - b)\) we get:

\[
L_N(1,1|i,j - i) + L_N(1,1|i,j - j) - L_N(1,1|i,j - i) - L_N(1,1|i,j - j) = (p - 2j)(L_N(1,1|i,j - h) + L_N(1,1|h,i - j) - L_N(1,1|i,j - h) - L_N(1,1|h,i + h)).
\] (8.7)

Computation shows that the following conjecture should hold.

**Conjecture 8.1.** The RDT \(8.5\) follows from the combination of the following relations: the seeded relations, the RDS \(8.1\) and \(8.2\), and the FDT \(8.3\) and \(8.4\).

### 8.3 Weight three.

Apparently there are \(N^2(N + 1)\) MPVs of weight 3 and level \(N\): for each choice \((i, j, k)\) with \(1 \leq i \leq N - 1, 0 \leq j, k \leq N - 1\) we have four MPVs of level \(N\):

\[
L_N(1,1,1|i,j,k), \quad L_N(1,2|i,j), \quad L_N(2,1|i,j,k), \quad L_N(3|k).
\]

For \(1 \leq i, j, k < N\) the FDS \(Z^*(y_1,i * (y_{1,j}y_1,k)) = Z^\text{III}(y_1,i^\text{M}(y_{1,j}y_1,k))\) yields

\[
L_N(\{1\}^3,i,j - k) + L_N(\{1\}^3,i,j - k) = L_N(\{1\}^3,i,j - k) + L_N(\{1\}^3,i,j - k)
\]

\[
= L_N(2,1,i,j,k) + L_N(2,1,i,j,k) + L_N(1,2,i,j,k) + L_N(1,2,i,j,k)
\]

\[
= L_N(\{1\}^3,i,j,k) + L_N(\{1\}^3,i,j,k) + L_N(\{1\}^3,i,j,k).
\] (8.8)

For \(1 \leq i, j < N\) the FDS \(Z^*(y_1,i * y_{2,j}) = Z^\text{III}(y_1,i^\text{M}y_{2,j})\) yields

\[
L_N(3,1|+j) + L_N(1,2,i,j,k) + L_N(2,1,i,j,k) = L_N(1,2,i,j,k) + L_N(2,1,i,j,k) + L_N(2,1,i,j,k).
\] (8.9)

Moreover, there are three ways to produce RDS. Since \(\beta(T) = T\) the first family of RDS come from \(Z^*(y_1,0 * (y_{1,i}y_{1,i+j})) = Z^\text{III}(y_1,0^\text{M}(y_{1,i}y_{1,i+j}))\) for \(1 \leq i \leq N - 1, 0 \leq j \leq N - 1\):

\[
y_1,0 * (y_{1,i}y_{1,i+j}) = y_1,0^\text{M}(y_{1,i}y_{1,i+j}) + y_1,i^\text{T}(y_1,0 * y_{1,j}) + y_2,iy_{1,i+j}
\]

\[
y = y_1,0y_1,iy_{1,i+j} + y_1,iy_{1,i}y_{1,i+j} + y_1,iy_{1,i+j}y_1,0 + y_1,iy_{1,i+j}y_2,iy_{1,i+j} + y_1,iy_{1,i+j}y_2,iy_{1,i+j} + y_1,iy_{1,i+j}y_2,iy_{1,i+j}
\]

On the other hand,

\[
y_1,0^\text{M}y_1,iy_{1,i+j} = y_1,0y_1,iy_{1,i+j} + y_1,iy_{1,0}y_{1,i+j} + y_1,iy_{1,i+j}y_1,0.
\]

Hence

\[
L_N(\{1\}^3,i,0,j) + L_N(\{1\}^3,i,j,0) + L_N(1,2,i,j,k) + L_N(2,1,i,j,k)
\]

\[
= L_N(\{1\}^3,i,0,j) + L_N(\{1\}^3,i,j,0) + L_N(\{1\}^3,i,j,0) - j).
\] (8.10)

The second family of RDS follow from \(\beta(Z^*(y_1,0 * y_{2,i})) = Z^\text{III}(y_1,0^\text{M}y_{2,i})\):

\[
y_1,0y_{2,i} + y_2,iy_{1,i} + y_3,i = y_1,0y_{2,i} + y_2,0y_{1,i} + y_2,iy_{1,0}
\]

which implies that

\[
L_N(2,1,i,0) + L_N(3,i) = L_N(2,1,i,0) + L_N(2,1,0,i).
\] (8.11)
Now we consider the last family of RDS. By the definition of shuffle product:

\[
y_{1,0} * y_{1,0} * y_{1,i} = (2y_{1,0}^2 + y_{2,0}) * y_{1,i}
\]

\[
= 2y_{1,0} (y_{1,0} * y_{1,i}) + 2y_{2,0} y_{1,i} + y_{2,0} * y_{1,i}
\]

\[
= 2y_{1,0} y_{1,i} + 2y_{1,0} y_{1,i}^2 + 2y_{1,0} y_{2,0} + 2y_{1,i} + 2y_{2,0} y_{1,i} + y_{2,0} * y_{1,i}.
\]

Applying \( \beta \circ Z^* \) and noticing that \( Z^I_{(0)}(T) = \zeta(2) \) we get

\[
(T^2 + \zeta(2))Z^I_{(1)}(T) = 2Z^I_{(0,0)}(T) + 2Z^I_{(1,1)(0,0,0)}(T) + 2Z^I_{(1,2)(0,0,0)}(T)
\]

\[
+ 2Z^I_{(1,1,0)(0,0,0,0)}(T) + 2Z^I_{(2,1)(0,0,0)}(T) + Z^I_{(2,0)}(T)Z^I_{(1)}(T). \quad (8.12)
\]

On the other hand by the definition of shuffle product

\[
\omega_0 \omega_0 \omega_0 y_{1,i} = 2\omega_0^2 \omega_i + 2\omega_0 \omega_i \omega_0 + 2\omega_i \omega_0^2
\]

\[
= 2y_{1,0}^2 y_{1,i} + 2y_{1,0} y_{1,i} y_{1,0} + 2y_{1,0} y_{1,i}^2
\]

Applying \( Z^I \) we get

\[
T^2 Z^I_{(1)}(T) = 2Z^I_{(1,1)(0,0,0)}(T) + 2Z^I_{(1,1,1)(0,0,0,0)}(T) + 2Z^I_{(1,1,1)(0,1,0)}(T). \quad (8.13)
\]

We further have

\[
Z^I_{(1,1)(0,0,0)}(T) = Z^I_{(1,1,1)(0,0,0,0)}(T) + 2Z^I_{(1,1,1)(0,1,0)}(T) - Z^I_{(1,1,1)(0,0,0,0)}(T)
\]

\[
= 2Z^I_{(1,1,1)(0,0,0)}(T) - Z^I_{(1,1,1)(0,1,0)}(T) - Z^I_{(1,1,1)(0,1,0)}(T) - Z^I_{(1,1,1)(0,1,0)}(T)
\]

where we have used the facts that

\[
Z^I_{(1,2)(0,0)}(T) = T Z^I_{(2,0)}(T) - Z^I_{(2,1)(0,0)}(T)
\]

\[
Z^I_{(1,1,1)(0,0,0)}(T) = T Z^I_{(1,1,1)(0,0,0,0)}(T) - Z^I_{(1,1,1)(0,1,0)}(T) - Z^I_{(1,1,1)(0,1,0)}(T) - Z^I_{(1,1,1)(0,1,0)}(T)
\]

Hence for \( 1 \leq i < N \) we have by subtracting (8.13) from (8.12)

\[
L_N(\{1\}^3, i, 0, 0) + L_N(2, 1, i, 0) + L_N(\{1\}^3, -i, 0) =
\]

\[
L_N(2, 1, i, -i) + L_N(2, 1, 0, i) + L_N(\{1\}^3, i, i, i) + L_N(\{1\}^3, 0, 0, 0, 0) + L_N(2, 1, i, 0) \quad (8.14)
\]

Setting \( j = 0 \) in (8.10) and subtracting from (8.14) we get

\[
L_N(\{1\}^3, i, -i, 0) = L_N(2, 1, i, -i) + L_N(2, 1, 0, i) + L_N(\{1\}^3, i, 0, 0) + L_N(2, 1, i, 0) \quad (8.15)
\]

### 8.4 Upper bound of \( d(w, N) \) by Deligne and Goncharov

By using the theory of motivic fundamental groups of \( \mathbb{P}^1 - \{0, \infty \} \cup \mu_N \), Deligne and Goncharov [11, 5.25] show that \( d(w, N) \leq D(w, N) \) where \( D(w, N) \) are defined by the formal power series

\[
1 + \sum_{w=1}^\infty D(w, N)t^w = \left\{ \begin{array}{ll}
(1 - t^2) - t^2, & \text{if } N = 1; \\
(1 - t^2) - t^2, & \text{if } N = 2; \\
(1 - \frac{t^N}{2} + \nu(N))t + (\nu(N) - 1)t^2, & \text{if } N \geq 3.
\end{array} \right. \quad (8.16)
\]

Here \( \varphi \) is the Euler’s totient function and \( \nu(N) \) is the number of distinct prime factors of \( N \). Set \( a = a(N) := \varphi(N)/2 + \nu(N) \) and \( b = b(N) := \nu(N) - 1 \). If \( N > 2 \) then we have

\[
\sum_{j=1}^\infty D(w, N)t^n = at + (a^2 - b)t^2 + (a^3 - 2ab)t^3 + (a^4 - 3a^2b + b^2)t^4 + (3ab^2 - 4a^3b + a^5)t^5 + \cdots
\]

We will compare the bound obtained by standard relations to \( D(w, N) \) in the next two sections.
9 Computational results in weight two

In this section we combine the analysis in the previous sections and the theory developed by Deligne and Goncharov [11] to present a detailed computation in weight two and level \( N \leq 49 \).

Let \( \mathcal{G} := \psi(\text{Lie } U_p) \) be the motivic fundamental Lie algebra (see [11] (5.12.2)) associated to the motivic fundamental group of \( \mathbb{P}^1 - \{0,1,\infty \} \cup \mu_N \). As pointed out in §6.13 of op. cit. one may safely replace \( \mathcal{G}(\mu_N)^{(i)} \) by \( \mathcal{G} \) throughout [14]. Then it follows from the proof of [11] 5.25 that if a variant of Grothendieck’s period conjecture (see 5.27(c) of op. cit.) is true, which we assume in the following, then

\[
d(2,N) = D(2,N) - \dim \ker(\beta_N),
\]

where \( \beta_N : \wedge^2 \mathcal{G}_{-1,-1} \longrightarrow \mathcal{G}_{-2,-2} \) is given by Ihara’s bracket \( \beta_N(a \wedge b) = \{a,b\} \) defined by (5.13.6) of op. cit. Here \( \mathcal{G}_{\star, \star} \) is the associated graded of the weight and depth gradings of \( \mathcal{G} \) (see [14] §2.1). Let \( k(N) := \dim \ker(\beta_N) \). Then

\[
\delta_1(N) := \dim \mathcal{G}_{-1,-1} = \varphi(N)/2 + \nu(N) - 1
\]

by [14] Thm. 2.1. Thus

\[
i(N) := \dim \text{Im}(\beta_N) = \delta_1(N)(\delta_1(N) - 1)/2 - k(N).
\]

Since \( \dim \mathcal{G}_{-2,-1} = \varphi(N)/2 \) if \( N > 2 \) and 0 otherwise the dimension of the degree 2 part of \( \mathcal{G} \) is

\[
\delta_2(N) := \dim \mathcal{G}_{-2,-1} + \dim \mathcal{G}_{-2,-2} = \begin{cases} 
i(N), & \text{if } N = 1 \text{ or } 2; \\ \varphi(N)/2 + i(N), & \text{if } N \geq 3.
\end{cases}
\]

Let \( sr(N) \) be the upper bound of \( \delta_2(N) \) obtained by the standard relations. This can be computed by the method described in [24]. Let \( SR(N) \) be the upper bound of \( d(2,N) \) similarly obtained by standard relations. In Table 1 we use MAPLE to provide the following data: \( k(N) \), \( sr(N) \), and \( SR(N) \). Then we can calculate \( \delta_1 \), \( \delta_2 \) and \( i(N) \) from (9.2) to (9.4). From (9.1) we can check the consistency by verifying

\[
sr(N) - \delta_2(N) = SR(N) - d(2,N) = SR(N) - D(2,N) + k(N)
\]

which gives the number of linearly independent non-standard relations (assuming Grothendieck’s period conjecture). To save space we use \( D = D(2,N) \) and \( d = d(2,N) \).

Remark 9.1. We now make the following observations in weight two case.

(a) If the level \( N \) is a prime then the standard relations provide all the \( \mathbb{Q} \)-linear relations under the assumption of a variant of Grothendieck’s period conjecture. This is proved in [24] Thm. 1.

(b) Notice that when \( p \geq 11 \) the vector space \( \ker \beta_p \) contains a subspace isomorphic to the space of cusp forms of weight two on \( X_1(p) \) which has dimension \( (p-5)(p-3)/24 \) (see [14] Lemma 2.3 & Theorem 7.8]). So it must contain another piece which has dimension \( (p-3)/2 \) since \( \dim(\ker \beta_p) = (p^2 - 1)/24 \) by [24] (5)). What is this missing piece?

(b) If \( N \) is a 2-power or a 3-power then \( D(2,N) \) should be sharp by the conjecture mentioned in (a). See Remark 6.3.

(c) If \( N \) has at least two distinct prime factors then \( D(2,N) \) seems to be sharp, though we don’t have any theory to support it.

(d) Suppose Grothendieck’s period conjecture is true. Then by [11] 5.27], (b) and (c) is equivalent to saying that the kernel of \( \beta_N \) is trivial if \( N \) is a 2-power or a 3-power, or has at least two distinct prime factors. We believe this condition on \( N \) for \( \beta_N \) to be trivial is necessary, too.

(e) If the level \( N \) is a \( p \)-power for some prime \( p \geq 5 \) then \( \beta_N \) is unlikely to be injective (the prime square case is proved in [24] Prop. 5.3)). We conjecture that non-standard relation doesn’t exist (i.e., \( SR(N) \) is sharp), though we only have verified the first two prime squares, \( N = 25 \) and \( N = 49 \).
| $N$  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 |
|-----|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|
| $\delta_1$ | 0 | 1 | 1 | 1 | 2 | 2 | 3 | 2 | 3 | 3 | 5 | 3 | 6 | 4 | 5 | 4 | 8 | 4 | 9 |
| $\delta_2$ | 0 | 1 | 1 | 1 | 2 | 2 | 4 | 3 | 6 | 5 | 10 | 5 | 14 | 9 | 14 | 10 | 24 | 9 | 30 |
| $sr$ | 0 | 1 | 1 | 1 | 2 | 2 | 4 | 4 | 6 | 6 | 10 | 8 | 14 | 12 | 16 | 16 | 24 | 19 | 30 |
| $D$ | 1 | 2 | 4 | 9 | 8 | 16 | 9 | 16 | 15 | 36 | 15 | 49 | 24 | 35 | 25 | 81 | 24 | 100 |
| $SR$ | 1 | 2 | 4 | 4 | 8 | 8 | 14 | 10 | 16 | 16 | 31 | 18 | 42 | 27 | 37 | 31 | 69 | 34 | 85 |
| $d$ | 1 | 2 | 4 | 4 | 8 | 8 | 14 | 9 | 16 | 15 | 31 | 15 | 42 | 24 | 35 | 25 | 69 | 24 | 85 |

$|N|$  | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 |
|$\delta_1$ | 5 | 7 | 6 | 11 | 5 | 10 | 7 | 9 | 7 | 14 | 6 | 15 | 8 | 11 | 9 | 13 | |
|$i$ | 10 | 21 | 15 | 33 | 10 | 40 | 21 | 36 | 21 | 56 | 15 | 65 | 28 | 55 | 36 | 78 | |
|$k$ | 0 | 0 | 0 | 0 | 0 | 22 | 0 | 5 | 0 | 0 | 0 | 35 | 0 | 40 | 0 | 0 | 0 | 0 | |
|$\delta_2$ | 14 | 27 | 20 | 44 | 14 | 50 | 27 | 45 | 27 | 70 | 19 | 80 | 36 | 65 | 44 | 90 | |
|$sr$ | 24 | 32 | 35 | 44 | 32 | 50 | 42 | 54 | 48 | 70 | 48 | 80 | 64 | 77 | 72 | 96 | |
|$D$ | 35 | 63 | 48 | 144 | 35 | 121 | 63 | 100 | 63 | 225 | 47 | 256 | 81 | 143 | 99 | 195 | |
|$SR$ | 45 | 68 | 58 | 122 | 53 | 116 | 78 | 109 | 84 | 190 | 76 | 216 | 109 | 158 | 127 | 201 | |
|$d$ | 35 | 63 | 48 | 122 | 35 | 116 | 63 | 100 | 63 | 190 | 47 | 216 | 81 | 143 | 99 | 195 | |

| $N$  | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 |
|-----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $\delta_1$ | 7 | 18 | 10 | 13 | 9 | 20 | 8 | 21 | 11 | 12 | 23 | 9 | 21 |
| $i$ | 21 | 96 | 45 | 78 | 36 | 210 | 28 | 133 | 55 | 78 | 66 | 161 | 36 | 175 |
| $k$ | 0 | 57 | 0 | 0 | 0 | 70 | 0 | 77 | 0 | 0 | 0 | 92 | 0 | 35 |
| $\delta_2$ | 27 | 114 | 54 | 90 | 44 | 140 | 34 | 154 | 65 | 90 | 77 | 184 | 44 | 196 |
| $sr$ | 72 | 114 | 89 | 112 | 96 | 140 | 96 | 154 | 120 | 144 | 132 | 184 | 128 | 196 |
| $D$ | 63 | 361 | 120 | 195 | 99 | 441 | 79 | 484 | 143 | 195 | 168 | 576 | 99 | 484 |
| $SR$ | 108 | 304 | 156 | 217 | 151 | 371 | 141 | 407 | 198 | 249 | 223 | 484 | 183 | 449 |
| $d$ | 63 | 304 | 120 | 195 | 99 | 371 | 79 | 407 | 143 | 195 | 168 | 484 | 99 | 449 |

Table 1: Upper bound of $d(2, N)$ obtained by standard relations and [11], 5.25.

** Remark 9.2.** In the three cases $(w, N) = (2, 8), (2, 10)$ and $(2, 12)$ we see that $d(w, N) > D(w, N)$. By numerical computation we conjecture that the bounds given by $D(w, N)$ are sharp in these cases and the following relations are the non-standard ones: let $L_N(-) = L_N(1, 1|-)$ and $L_N^{(2)}(-) = L_N(2|-)$, then

$$37L_8(1, 1) = 34L_8^{(2)}(5) + 112L_8(3, 1) + 11L_8(3, 0) + 37L_8^{(2)}(1) - 2L_8(2, 6)$$
$$+ 3L_8(7, 3) - 111L_8(5, 7) + 38L_8(7, 7) - 8L_8(5, 5), \quad \text{(9.5)}$$

$$7L_{10}(5, 2) = 7L_{10}^{(2)}(1) + 265L_{10}^{(2)}(7) - 7L_{10}(2, 5) - 467L_{10}(4, 2) + 467L_{10}(8, 6)$$
$$+ 14L_{10}(5, 6) + 64L_{10}(9, 8) - 164L_{10}(9, 4) + 166L_{10}(7, 9)$$
$$- 260L_{10}(8, 1) - 66L_{10}(3, 9) - 7L_{10}(6, 9) + 7L_{10}(6, 5), \quad \text{(9.6)}$$

$$L_{12}(8, 7) = 5L_{12}^{(2)}(5) + 8L_{12}(8, 10) - 6L_{12}(10, 11) - 8L_{12}(9, 11) + L_{12}(10, 9)$$
$$- 15L_{12}(8, 1) + 5L_{12}(9, 10) + 5L_{12}(6, 1) - L_{12}(1, 1)$$
$$+ 6L_{12}(8, 11) - 11L_{12}(6, 11) + 8L_{12}(8, 3) - L_{12}(11, 8), \quad \text{(9.7)}$$

$$60L_{12}(8, 11) = 38L_{12}(8, 7) + 348L_{12}(10, 11) + 502L_{12}(9, 11) - 492L_{12}(10, 9)$$
$$+ 600L_{12}(8, 1) - 552L_{12}(9, 10) - 154L_{12}(11, 10) + 20L_{12}(6, 1)$$
$$+ 261L_{12}(6, 11) - 502L_{12}(8, 3) + 221L_{12}(11, 8) - 319L_{12}(8, 10), \quad \text{(9.8)}$$

19
\[221L_{12}(1, 1) = 1854L_{12}(8, 10) + 562L_{12}(8, 7) - 1018L_{12}(10, 11) - 2416L_{12}(9, 11) + 319L_{12}(10, 9) - 4270L_{12}(8, 1) + 2293L_{12}(9, 10) + 956L_{12}(11, 10) + 1110L_{12}(6, 1) + 2416L_{12}(8, 11) - 3305L_{12}(6, 11) + 2416L_{12}(8, 3). \] (9.9)

**Definition 9.3.** We call the level \( N \) standard if either (i) \( N = 1, 2 \) or 3, or (ii) \( N \) is a prime power \( p^n \) \((p \geq 5)\). Otherwise \( N \) is called non-standard.

When \( N \) is a non-standard level we find that very often there are non-standard relations among MPVs. For examples, the five relations in Remark 9.2 are discovered only through numerical computation. But are the standard relations enough to produce all the linear relations when \( N \) is standard? In weight two, when \( N \) is a prime the answer is affirmative if one assumes a variant of Grothendieck’s period conjecture [24]. Computations above give strong support for it and, in fact, is the primary motivation of it.

### 10 Computational results in other weights

In this last section we briefly discuss our results in weight 3,4 and 5. Since the computational complexity increases exponentially with weight we cannot do as many cases as we have done in weight two.

Combining the FDS \((8.8), (8.9), \) RDS \((8.10)-(8.15), \) and the seeded relations \((4.3)\) we have verified the following facts by MAPLE: \( d(3, 1) = 1, \) \( d(3, 2) \leq 3, \) \( d(3, 3) \leq 8 \ldots \) We have done similar computation in other small weight and low level cases and listed the results in Table [2].

We list some values of \( D(w, N) \) in Table 2 to compare with the bound \( SR(w, N) \) obtained by standard relations.

| \( N \) | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
|-------|---|---|---|---|---|---|---|---|---|----|----|----|----|
| \( SR(3, N) \) | 1 | 3 | 8 | 9 | 22 | 23 | 50 | 38 | 67 | 70 | 157 | 94 | 246 |
| \( D(3, N) \) | 1 | 4 | 16 | 32 | 144 | 243 | 1024 | 243 | 1024 | 780 | 7776 | 780 | 16807 |
| \( SR(4, N) \) | 1 | 5 | 16 | 21 | 61 | 69 | \ | \ | \ | \ | \ | \ |
| \( D(4, N) \) | 1 | 5 | 16 | 16 | 81 | 55 | 256 | 81 | 256 | 209 | 1296 | 209 | 2401 |
| \( SR(5, N) \) | 2 | 8 | 32 | 32 | 243 | 144 | 1024 | 243 | 1024 | 780 | 7776 | 780 | 16807 |

Table 2: Upper bound of \( d(w, N) \) obtained by standard relations and [11, 5.25].

**Remark 10.1.** Note that \( d(3, 4) = D(3, 4) + 1 \). By numerical computation we find the following non-standard relation:

\[
\begin{align*}
5L_4(1, 2|2, 3) &= 46L_4(1, 1|1, 0, 0) - 7L_4(1, 1|2, 2, 1) - 13L_4(1, 1|1, 1, 1) + 13L_4(1, 2|3, 1) \\
- L_4(1, 1|3, 2, 0) + 25L_4(1, 1|3, 0, 0) - 8L_4(1, 1|1, 1, 2) + 18L_4(2, 1|3, 0),
\end{align*}
\] (10.1)

Recently, we prove that by using the octahedral symmetry of \( \mathbb{P}^1 - (\{0, \infty\} \cup \mu_4) \) one can deduce equation (10.1) (see [24]).

From the available data in Table 2 we can formulate the following conjecture.

**Conjecture 10.2.** Let \( N = p \) be a prime \( \geq 5 \). Then

\[
d(3, p) \leq \frac{p^3 + 4p^2 + 5p + 14}{12}.
\]

Moreover, equality hold if standard relations produce all the linear relations.
We obtained this conjecture under the belief that the upper bound of \( d(3,p) \) produced by the standard relations should be a polynomial of \( p \) of degree 3. Then we find the coefficients by the bounds of \( d(3,p) \) for \( p = 5, 7, 11, 13 \) in Table 2.

When \( w > 2 \) it’s not too hard to improve the bound of \( d(w,p) \) given in [11, 5.25] by the same idea as used in the proof of [11, 5.24] (for example, decrease the bound by \( (p^2 - 1)/24 \)). But they are often not the best. We conclude our paper with the following conjecture.

**Conjecture 10.3.** If \( N \) is a standard level then the standard relations always provide the sharp bounds of \( d(w,N) \), namely, all linear relations can be derived from the standard ones. If \( N \) is a non-standard level then the bound in [11, Cor. 5.25] is sharp and the non-standard relations exist in \( MPV(w,N) \) for all \( w \geq 3 \) (and in \( MPV(2,N) \) if \( N \geq 10 \)).

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