Identities arising from coproducts on multiple zeta values and multiple polylogarithms

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Dedicated to

My mother, Joyce,
who didn't live to see
this thesis finished

Joyce Charlton
8 March 1953 – 24 June 2016

Also to

My sister, Susan

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Abstract: In this thesis we explore identities which can be proven on multiple zeta values using the derivation operators D_r from Brown's motivic MZV framework. We then explore identities which occur on multiple polylogarithms by way of the symbol map $\mathcal{S}$, and the multiple polylogarithm coproduct Δ.

On multiple zeta values, we consider Borwein, Bradley, Broadhurst, and Lisoněk's cyclic insertion conjecture about inserting blocks of $\{2\}^{a_i}$ between the arguments of $\zeta(\{1,3\}^n)$. We generalise this conjecture to a much broader setting, and give a proof of a symmetrisation of this generalised cyclic insertion conjecture. This proof is by way of the block-decomposition of iterated integrals introduced here, and Brown's motivic MZV framework. This symmetrisation allows us to prove (or to make progress towards) various conjectural identities, including the original cyclic insertion conjecture, and Hoffman's $2\zeta(3,3,\{2\}^n) - \zeta(3,\{2\}^n,1,2)$ identity. Moreover, we can then generate unlimited new conjectural identities, and give motivic proofs of their symmetrisations.

We then consider the task of relating weight 5 multiple polylogarithms. Using the symbol map, we determine all of the symmetries and functional equations between depth 2 and between depth 3 iterated integrals with 'coupled-cross ratio' arguments $[\operatorname{cr}(a,b,c,d_1),\ldots,\operatorname{cr}(a,b,c,d_k)]$. We lift the identity for $I_{4,1}(x,y)+I_{4,1}(\frac{1}{x},\frac{1}{y})$ to an identity holding exactly on the level of the symbol and prove a generalisation of this for $I_{a,b}(x,y)$. Moreover, we further lift the subfamily $I_{n,1}$ to a candidate numerically testable identity using slices of the coproduct.

We review Dan's reduction method for reducing the iterated integral $I_{1,1,\ldots,1}$ to a sum in $\leq n-2$ variables. We provide proofs for Dan's claims, and run the method in the case $I_{1,1,1,1}$ to correct Dan's original reduction of $I_{1,1,1,1}$ to $I_{3,1}$ and I_4. We can then compare this with another reduction to find $I_{3,1}$ functional equations, and their nature. We then give a reduction of $I_{1,1,1,1,1}$ to $I_{3,1,1}$, $I_{3,2}$ and I_5, and indicate how one might be able to further reduce to $I_{3,2}$ and I_5.

Lastly, we use and generalise an idea suggested by Goncharov at weight 4 and weight 5. We find Li_n terms when certain Li_2, Li_3 and Li_4 functional equations are substituted into the arguments of symmetrisations of $I_{m,1}(x,y)$. By expanding $I_{m,1}(\mathrm{Li}_k \text{ equation}, \mathrm{Li}_\ell \text{ equation})$ in two different ways we obtain functional equations for Li_5 and Li_6. We make some suggestions for how this might work at weight 7 and weight 8 giving a potential route to Li_7 and Li_8 functional equations.

Declaration

The work in this thesis is based on research carried out in the Pure Mathematics Group, Department of Mathematical Sciences, Durham University, United Kingdom. No part of this thesis has been submitted elsewhere for any other degree or qualification and it is all my own work unless referenced to the contrary in the text.

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Contents

Chapter 1

(Motivic) multiple zeta values

We review the basic definitions and theory surrounding multiple zeta values, including some of their history. The definition of an MZV (Definition 1.1.1) is motivated by considering products of Riemann zeta values. We consider Euler's results on evaluating $\zeta(2k)$ (Theorem 1.1.6) and on reducing the double zeta values $\zeta(1, k)$ to polynomials in $\zeta(n)$'s (Theorem 1.1.8). We see how to represent MZV's as iterated integrals (Proposition 1.1.16), and how multiplying them gives a shuffle product operation, which complements the stuffle product obtained by multiplying the series representation (Section 1.1.4). We then consider some reasons for the interest in MZV's, particularly questions dealing with the transcendentality aspects that have so far defied solution (Section 1.1.5).

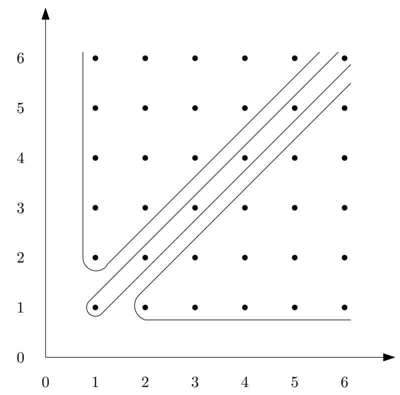
Then we turn to the idea of a motivic MZV, originally defined by Goncharov (Section 1.2.2) and extended by Brown. Motivic MZV's provide a purely algebraic lifting of the usual MZV's, that eliminates transcendentality problems from the start. We review Goncharov's Hopf algebra of motivic iterated integrals (Section 1.2.1), and see how the coproduct (Theorem 1.2.1) provides new insight into the structure of the usual iterated integrals, and MZV's (Proposition 1.2.6). Finally we introduce Brown's motivic MZV framework (Section 1.2.3), and the combinatorial tools it provides to algorithmically decompose MZV's. These combinatorial tools include the family of derivations D_r (Definition 1.2.12), and Brown's characterisation of the kernel of this family $\ker D_{<N}$ (Theorem 1.2.15).

1.1 Multiple zeta values

1.1.1 Definitions

Multiple zeta values (which we may henceforth abbreviate as MZV's) are an intriguing class of real numbers, first studied by Euler in the special case of *double* zeta values. Systematic study of the general case begins with Hoffman [Hof92]. The multiple zeta *function* is a generalisation of the Riemann zeta function to a k-tuple of arguments, but for number theoretic reasons, we are mainly interested in the case where the arguments are positive integers.

The definition of a multiple zeta value can be somewhat motivated by considering what happens when we multiply the Riemann zeta values $\zeta(a)$ and $\zeta(b)$. This will involve a sum over the first quadrant $\mathbb{Z}_{>0} \times \mathbb{Z}_{>0}$, which can then be decomposed into a sum over a diagonal piece, an upper trianglar piece and a lower triangular piece.



We find

$$\begin{aligned}\zeta(a)\zeta(b) &= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty} \frac{1}{n^a m^b} \\ &= \left(\sum_{n<m} + \sum_{n=m} + \sum_{n>m}\right) \frac{1}{n^a m^b} \\ &=: \zeta(a,b) + \zeta(a+b) + \zeta(b,a)\,.\end{aligned}$$

Now we give the more general definition of a multiple zeta value.

Definition 1.1.1 (Multiple zeta values)**.** Let $s_1, s_2, \ldots, s_k \in \mathbb{C}$. Then the multiple zeta function $\zeta(s_1, s_2, \ldots, s_k)$ is defined as follows

$$\zeta(s_1, s_2, \ldots, s_k) \coloneqq \sum_{0<n_1<n_2<\cdots<n_k} \frac{1}{n_1^{s_1} n_2^{s_2} \cdots n_k^{s_k}}\,.$$

Taking $s_1, s_2, \ldots, s_k$ to be integers in $\mathbb{Z}_{>0}$, we obtain the *multiple zeta value* $\zeta(s_1, s_2, \ldots, s_k)$.

Warning 1.1.2. There are two competing conventions about the index of summation. Some take $n_1 > n_2 > \cdots > n_k > 0$, rather than the index $0 < n_1 < n_2 < \cdots < n_k$ used above. This essentially has the effect of reversing the arguments to the multiple zeta function, so no information is lost. However, one must be aware of which convention is in use, especially when numerically checking identities.

Multiple zeta values can be viewed as special values of the multiple polylogarithms, to be introduced later in Chapter 3. We won't need this point of view, except for the fact that multiple polylogarithms (and hence MZV's) can be written as iterated integrals.

Auxiliary to the definition of an MZV are the notions of *depth* and *weight*.

Definition 1.1.3 (MZV weight, MZV depth)**.** Given an MZV $\zeta(s_1, s_2, \ldots, s_k)$ we define the following.

- The sum of the arguments $s_1 + s_2 + \cdots + s_k$ is called the *weight* of $\zeta(s_1, s_2, \ldots, s_k)$.
- The number k of its arguments is called the *depth* of $\zeta(s_1, s_2, \ldots, s_k)$.

Proposition 1.1.4. *Suppose* $s_1, s_2, \ldots, s_k \in \mathbb{Z}_{>0}$*. Then the MZV* $\zeta(s_1, s_2, \ldots, s_k)$ *is* convergent *if and only if* $s_k > 1$*.*

Proof sketch: Since the series consists only of positive terms, it converges if and only if it converges absolutely. In particular the summation order does not matter.

'⇒': If $s_k = 1$, then by taking the subseries where $n_i = i$, for $i = 1, \ldots, k-1$, we obtain

$$\zeta(s_1, \ldots, s_{k-1}, 1) \geq \frac{1}{1^{s_1} 2^{s_2} \cdots (k-1)^{s_{k-1}}} \sum_{n_k = k}^{\infty} \frac{1}{n_k^1} \,,$$

but the latter series is (a multiple of a tail of) the harmonic series. In particular this diverges. Hence $\zeta(s_1, \ldots, s_{k-1}, 1)$ is divergent by comparison. So by the contrapositive, $\zeta(s_1, s_2, \ldots, s_k)$ is convergent implies $s_k > 1$.

'⇐': Suppose that $s_k \geq 2$. Let $I = \{\, 1 \leq i < k \mid s_i > 1 \,\}$, and $J = \{\, 1 \leq i < k \mid s_i = 1 \,\}$. By fixing some n_k, we have that

$$\sum_{0 < n_1 < \cdots < n_{k-1} < n_k} \frac{1}{n_1^{s_1} \cdots n_{k-1}^{s_{k-1}}} \leq \sum_{n_1, \ldots, n_{k-1} = 1}^{n_k} \frac{1}{n_1^{s_1} \cdots n_{k-1}^{s_{k-1}}} = \prod_{i=1}^{k-1} \sum_{n_i = 1}^{n_k} \frac{1}{n_i^{s_i}} \,.$$

For the terms $i \in I$ where $s_i > 1$, we have that

$$\sum_{n_i = 1}^{n_k} \frac{1}{n_i^{s_i}} < \sum_{n_i = 1}^{\infty} \frac{1}{n_i^{s_i}} = \zeta(s_i) \,.$$

For the terms $i \in J$, where $s_i = 1$, we can apply the integral test to obtain the upper bound

$$\sum_{n_i = 1}^{n_k} \frac{1}{n_i^1} < \log(n_k) + 1 \,.$$

So we obtain

$$\zeta(s_1, \ldots, s_k) \leq \prod_{i \in I} \zeta(s_i) \sum_{n_k = 1}^{\infty} \frac{(\log(n_k) + 1)^{\#J}}{n_k^{s_k}} \,.$$

Since

$$\lim_{n \to \infty} \frac{1 + \log(n)}{n^\epsilon} = 0 \,,$$

for any $\epsilon > 0$, we can take $\epsilon = \frac{1}{2}$, so that

$$\lim_{n \to \infty} \frac{(\log(n_k) + 1)^{\#J}}{n_k^{1/2}} = \left(\lim_{n_k \to \infty} \frac{\log(n_k) + 1}{n_k^{\frac{1}{2\#J}}} \right)^{\#J} = 0 \,.$$

This means that the sequence is bounded, and so there is a constant C such that

$$(\log(n_k) + 1)^{\#J} < C n_k^{\frac{1}{2}} \,,$$

for all n_k.

Plugging this back into the upper bound for $\zeta(s_1, \ldots, s_k)$ gives us that

$$\zeta(s_1, \ldots, s_k) \leq \prod_{i \in I} \zeta(s_i) \sum_{n_k=1}^{\infty} \frac{(\log(n_k)+1)^{\#J}}{n_k^{s_k}} < C \prod_{i \in I} \zeta(s_i) \sum_{n_k=1}^{\infty} \frac{1}{n_k^{s_k - 1/2}} \,.$$

But this latter series is convergent since $s_k \geq 2$ means that $s_k - 1/2 > 1$.

Combining both directions shows that $\zeta(s_1, \ldots, s_k)$ converges iff $s_k > 1$, as claimed. □

1.1.2 Euler's results

1.1.2.1 Evaluation of ζ(even)

Perhaps one of Euler's most famous results is the successful evaluation of $\zeta(2)$, and by extension all $\zeta(2k)$. This leads to an answer to the question of the algebraic nature of ζ(even), namely ζ(even) is a transcendental number.

To state Euler's result, we first need to define the Bernoulli numbers B_{2n}.

Definition 1.1.5 (Bernoulli numbers)**.** The *Bernoulli numbers* B_{2n} are defined by the following generating series

$$\frac{z}{e^z - 1} =: \sum_{k=0}^{\infty} \frac{B_k}{k!} z^k \,.$$

Theorem 1.1.6 (Euler, [Eul43])**.** *Let $k \in \mathbb{Z}_{>0}$. The following evaluation of $\zeta(2k)$ holds.*

$$\zeta(2k) = \frac{(2\pi)^{2k}(-1)^{k+1} B_{2k}}{2(2k)!} \,. \tag{1.1.1}$$

In particular, $\zeta(2k)$ is a rational multiple of π^{2k}.

Proof sketch (not Euler's proof): The following series converges to $\pi z \cot(\pi z)$

$$\pi z cot(\pi z) = 1 + 2z^2 \sum_{n=1}^{\infty} \frac{1}{z^2 - n^2} \,.$$

But $\pi z \cot(\pi z)$ is holomorphic at 0, so we can use this series to find the power series expansion of $\pi z \cot(\pi z)$ at $z = 0$. For $|z| < 1$, we obtain

$$\begin{aligned} \pi z \cot(\pi z) &= 1 + 2z^2 \sum_{n=1}^{\infty} \frac{1}{z^2 - n^2} \\ &= 1 - 2z^2 \sum_{n=1}^{\infty} \frac{1}{n^2(1 - (z/n)^2)} \\ &= 1 - 2z^2 \sum_{n=1}^{\infty} \left(\sum_{k=0}^{\infty} \left(\frac{z}{n}\right)^{2k} \right) \,. \end{aligned}$$

We can interchange the order of summation to obtain

$$= 1 - 2 \sum_{k=0}^{\infty} \left(\sum_{n=1}^{\infty} \frac{1}{n^{2k+2}} \right) z^{2k+2}$$

$$= 1 - 2\sum_{k=1}^{\infty} \zeta(2k) z^{2k} \,. \tag{1.1.2}$$

On the other hand, we can write

$$\pi z \cot(\pi z) = \pi \mathrm{i} z \frac{e^{2\pi \mathrm{i} z} + 1}{e^{2\pi \mathrm{i} z} - 1} = \frac{(2\pi \mathrm{i} z)}{e^{2\pi \mathrm{i} z} - 1} + \pi \mathrm{i} z \,.$$

Expanding this out using the power series definition from Definition 1.1.5, we obtain

$$= 1 + \sum_{k=1}^{\infty} \frac{B_k}{(k!)} (2\pi \mathrm{i} z)^k \,. \tag{1.1.3}$$

Comparing coefficients between Equation 1.1.2 and Equation 1.1.3 leads to

$$-2\zeta(2k) = \frac{B_{2k}}{(2k)!} (2\pi \mathrm{i})^{2k} \,,$$

which can be rearranged to give Equation 1.1.1. □

From this evaluation, we can conclude that $\zeta(2k)$ is irrational, and in fact transcendental, using Linderman's theorem on the transcendentality of π. Moreover, since π is transcendental, all $\zeta(2k)$ are $\mathbb{Q}$-linearly independent. Euler, however, was not able to evaluate $\zeta(3)$, nor any other $\zeta(\text{odd})$, and the algebraic nature of $\zeta(\text{odd})$ still remains largely a mystery.

1.1.2.2 $\zeta(1,2) = \zeta(3)$, and reduction of double zeta values

The earliest results on genuine *multiple* zeta values date back to Euler's investigations of double zeta values, i.e. those where the depth is 2. His goal was to reduce these double zeta values to polynomials in $\zeta(n)$'s. One of the simplest examples of this reduction is the following result of Euler.

Proposition 1.1.7 (Euler, [Eul75])**.** *The following identity relates $\zeta(3)$ and $\zeta(1,2)$.*

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

Proof. There are many, many different proofs of this identity ranging from direct proofs involving manipulating series, to subtler proofs which establish generalisations for q-multiple zeta values, or for Witten multiple zeta values. Details of these proofs and more can be found in [BB06]. Perhaps the quickest proof, which appears at the start of section 2 of [BB06], and is credited to Steinberg [Ste52], is the following.

Consider

$$S \coloneqq \sum_{n,k=1}^{\infty} \frac{1}{nk(n+k)} \,.$$

We can write

$$\frac{1}{nk(n+k)} = \frac{1}{n^2}\left(\frac{1}{k} - \frac{1}{n+k}\right) \,,$$

to obtain

$$S = \sum_{n,k=1}^{\infty} \frac{1}{n^2} \left(\frac{1}{k} - \frac{1}{n+k} \right) = \sum_{n=1}^{\infty} \frac{1}{n^2} \left(\sum_{k=1}^{n} \frac{1}{k} \right),$$

since the inner sum telescopes. Then by splitting the k sum into $k < n$ and $k = n$ terms, this is equal to

$$\begin{aligned} &= \sum_{n=1}^{\infty} \sum_{k=1}^{n-1} \frac{1}{n^2 k} + \sum_{n=1}^{\infty} \frac{1}{n^3} \\ &= \zeta(1,2) + \zeta(3) . \end{aligned}$$

Alternatively, one can write

$$\frac{1}{nk(n+k)} = \left(\frac{1}{n} + \frac{1}{k} \right) \frac{1}{(n+k)^2},$$

to obtain

$$S = \sum_{n,k=1}^{\infty} \left(\frac{1}{n} + \frac{1}{k} \right) \frac{1}{(n+k)^2} = 2 \sum_{n,k=1}^{\infty} \frac{1}{n(n+k)^2} .$$

This is by using the $n \leftrightarrow k$ symmetry of the two terms in the first expression. Then by changing variables, $\ell = n + k$, we obtain

$$= 2 \sum_{0<n<\ell} \frac{1}{n\ell^2} = 2\zeta(1,2) .$$

Comparing these two expressions for S gives immediately

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

as claimed. □

This is an instance of the so-called *duality* of MZV's. Once the idea of duality is introduced more generally below, this identity will be an effortless one-line result. However, Euler provided a generalisation of this $\zeta(1,2) = \zeta(3)$ result in a different direction.

Theorem 1.1.8 (Euler, [Eul75])**.** *For $m \geq 2 \in \mathbb{Z}$, the following reduction, of the double zeta value $\zeta(1,m)$ to a polynomial in Riemann zeta values $\zeta(n)$, holds.*

$$2\zeta(1,m) = m\zeta(m+1) - \sum_{j=1}^{m-2} \zeta(j+1)\zeta(m-j) .$$

Although Euler's goal was to reduce all depth 2 MZV's to polynomials in Riemann zeta values $\zeta(n)$, he did not succeed. For example, no reduction for $\zeta(3,5)$ appears to exist, although the fact that $\zeta(3,5)$ is 'irreducible' is still only conjectural. We will revisit the question of the irreducibility of $\zeta(3,5)$ in Proposition 1.2.6, where we sketch Goncharov's proof of this result on *motivic MZV's*.

1.1.3 Iterated integrals

As already remarked, iterated integrals will give us another way of writing MZV's. This integral representation enriches the algebraic structure of MZV's, and will play an important role in the motivic framework introduced first by Goncharov, and subsequently improved by Brown.

Definition 1.1.9. Write

$$\omega(a_i) = \frac{\mathrm{d}t}{t - a_i}$$

for the unique differential form of degree 1, holomorphic on $\mathbb{P}^1(\mathbb{C}) \setminus \{ a_i \}$, which has a pole of order 1 and residue $+1$ at a_i.

Definition 1.1.10 (Chen iterated integral, [Che77])**.** Let $x_0, \ldots, x_{m+1}$ be complex numbers. Then a *(Chen) iterated integral* is defined by

$$\begin{aligned} I_\gamma(x_0; x_1, \ldots, x_m; x_{m+1}) &\coloneqq \int_{\Delta_\gamma} \frac{\mathrm{d}t_1}{t_1 - x_1} \wedge \cdots \wedge \frac{\mathrm{d}t_m}{t_m - x_m} \\ &= \int_{\Delta_\gamma} \omega(x_1)(t_1) \wedge \cdots \wedge \omega(x_m)(t_m) \,, \end{aligned}$$

where γ is a path from x_0 to x_{m+1} in $\mathbb{C} \setminus \{x_1, \ldots, x_m\}$, and the region of integration Δ_γ consists of all m-tuples $(\gamma(t_1), \ldots, \gamma(t_m))$, with $t_1 \leq t_2 \leq \cdots \leq t_m$.

The integral $I_\gamma(x_0; x_1, \ldots, x_m; x_{m+1})$ depends on the choice of path γ between x_0 and x_{m+1}, so it is a *multivalued* function of $x_0, \ldots, x_{m+1}$.

Remark 1.1.11. We will often drop γ from the iterated integral notation $I_\gamma(x_0; x_1, \ldots, x_m; x_{m+1})$ and simply write $I(x_0; x_1, \ldots, x_m; x_{m+1})$ instead. In the case of MZV's, this is because there is a standard choice for the path γ, (Proposition 1.1.16). In the case of multiple polylogarithms (Chapter 3) we will be more interested in the algebraic properties of $I(x_0; x_1, \ldots, x_m; x_{m+1})$, rather than the analytic properties (when computing the coproduct (Theorem 1.2.1), or the symbol (Section 3.3.2), say).

Remark 1.1.12. We may also use the following notation

$$\begin{aligned} I(x_0; x_1, \ldots, x_m; x_{m+1}) &= \int_{x_0}^{x_{m+1}} \omega(a_1) \circ \cdots \circ \omega(a_n) \\ &= \int_{x_0 \leq t_1 \leq \cdots \leq t_m \leq x_{m+1}} \omega(a_1)(t_1) \wedge \cdots \wedge \omega(a_n)(t_n) \end{aligned}$$

to write these integrals.

These integrals deserve the name *iterated* integrals because we can integrate each variable t_i one-by-one in a recursive way

$$\begin{aligned} &\int_{x_0}^{x_{n+1}} I(x_0; x_1, \ldots, x_{n-1}; t) \omega(a_i)(t) \\ &= \int_{x_0}^{x_{n+1}} \left(\int_{x_0 \leq t_1 \leq t_2 \leq \cdots \leq t_{n-1} \leq t_n} \omega(a_1) \circ \cdots \circ \omega(a_{n-1}) \right) \omega(a_n) \\ &= \int_{x_0 \leq t_1 \leq t_2 \leq \cdots \leq t_n \leq x_{n+1}} \omega(a_1) \circ \cdots \circ \omega(a_n) \\ &= I(x_0; x_1, \ldots, x_n; x_{n+1}) \,. \end{aligned}$$

These integrals are convergent if $x_0 \neq x_1$, and $x_n \neq x_{n+1}$. Otherwise they are divergent.

These integrals satisfy a number of standard, and well known properties.

Property 1.1.13 (Chen, [Che77]). The iterated integrals $I_\gamma(x_0; x_1, \ldots, x_n, x_{n+1})$ satisfy the following properties.

i) (Equal boundaries) If $n \geq 1$, $x_0 = x_{m+1}$, and γ is the trivial path from x_0 to $x_{m+1} = x_0$, then

$$I_\gamma(x_0; x_1, \ldots, x_n; x_{n+1}) = 0\,.$$

ii) (Unit/Empty integral) For any x_0, x_1, we have $I_\gamma(x_0; x_1) = 1$.

iii) (Path composition) Let $y \in \mathbb{C}$ be fixed. Let α be a path from x_0 to y, and β be a path from y to x_{m+1}. Denote by $\alpha\beta$ the composite path obtained by following α and then following β. Then

$$\begin{aligned}&I_{\alpha\beta}(x_0; x_1, \ldots, x_n; x_{n+1}) = \\ &\sum_{k=0}^{n} I_\alpha(x_0; x_1, \ldots, x_k; y) I_\beta(y; x_{k+1}, \ldots, x_n; x_{n+1})\,.\end{aligned}$$

iv) (Shuffle product) Two iterated integrals, with the same limits, can be multiplied using the shuffle product (explained fully below)

$$I_\gamma(a; x_1, \ldots, x_m; b) I_\gamma(a; x_{m+1}, \ldots, x_{m+n}; b) = I_\gamma(a; (x_1 \cdots x_m) \sqcup\!\sqcup (x_{m+1} \cdots x_{m+n}); b)\,.$$

v) (Reversal of paths) Let γ be a path from x_0 to x_{n+1}, and denote by γ^{-1} the reversed path. Then reversing the path of integration gives

$$I_\gamma(x_0; x_1, \ldots, x_n; x_{n+1}) = (-1)^n I_{\gamma^{-1}}(x_{n+1}; x_n, \ldots, x_1; x_0)\,.$$

vi) (Functoriality) Given a (piecewise) smooth map $f\colon \mathbb{C} \to \mathbb{C}$, we have

$$I_\gamma(x_0; x_1, \ldots, x_m; x_{m+1}) = \int_{\Delta_{f(\gamma)}} f^* \frac{\mathrm{d}t_1}{t_1 - x_1} \wedge \cdots \wedge f^* \frac{\mathrm{d}t_m}{t_m - x_m}\,.$$

In particular, under $f(t) = 1 - t$, we obtain

$$I_\gamma(x_0; x_1, \ldots, x_m; x_{m+1}) = I_{1-\gamma}(1 - x_0; 1 - x_1, \ldots, 1 - x_m; 1 - x_{m+1})\,.$$

Remark 1.1.14. The definition of an iterated integral, and the above properties, hold more generally. One does not need to restrict to the particular differential forms

$$\omega(a_i) \coloneqq \frac{\mathrm{d}t}{t - a_i}\,.$$

Any family of differential forms $\omega_1, \ldots, \omega_k$ will work; as long as the path γ of integration avoids the poles of the ω_i's, the resulting integral is well-defined. In particular, in Chapter 5, we shall generalise $\omega(a_i)$ to a form $\omega(a_i, x)$, which agrees with $\omega(a_i)$ when $x = \infty$.

Definition 1.1.15 (Shuffle product)**.** Given two words $w = a_1 \cdots a_m$ and $v = a_{m+1} \cdots a_{m+n}$ over some alphabet, the *shuffle product* $w \sqcup\!\sqcup v$ is defined as follows.

$$w \sqcup\!\sqcup v = \sum_{\sigma \in S_{m,n}} a_{\sigma(1)} \cdots a_{\sigma(m+n)} \,,$$

where $S_{m,n}$ is the set of (m,n)-shuffles

$$S_{m,n} \coloneqq \{\ \sigma \in S_{n+m} \mid\ \sigma(1) < \sigma(2) < \cdots < \sigma(m) \text{ and } \sigma(m+1) < \sigma(m+2) < \cdots < \sigma(m+n)\ \} \,.$$

Alternatively, the shuffle product can be defined recursively by the following conditions.

i) For any word w, $1 \sqcup\!\sqcup w = w \sqcup\!\sqcup 1 = w$, where 1 is the empty word.

ii) For any words w_1, w_2, and letters a, b, we have

$$(aw_1) \sqcup\!\sqcup (bw_2) = a(w_1 \sqcup\!\sqcup (bw_2)) + b((aw_1) \sqcup\!\sqcup w_2) \,.$$

The idea to keep in mind with the shuffle product is that the letters of the words w and v are permuted together, but individual letters of w remain in order, as do the individual letters of v. The words w and v are *riffle* shuffled, like a deck of cards.

According to Zagier [Zag94], Kontsevich was the first to notice how MZV's can be written using these iterated integrals.

Proposition 1.1.16 (Kontsevich)**.** *Let $\zeta(s_1, \ldots, s_k)$ be an MZV. Then*

$$\zeta(s_1, \ldots, s_k) = (-1)^k I(0; 1, \{0\}^{s_1 - 1}, \ldots, 1, \{0\}^{s_k - 1}; 1) \,,$$

where here $\{0\}^s \coloneqq \underbrace{0, \ldots, 0}_{s \text{ times}}$ means the string formed by repeating 0 a total of s times. (Here the path of integration is the straight line path from 0 to 1.)

Proof. This is actually a special case of a corresponding statement for multiple polylogarithms. The sketch proof of the general case is presented in Theorem 3.1.5. Essentially, it involves expanding out the integrand as geometric series, and integrating term by term. □

1.1.4 Algebraic structure of MZV's and standard relations

Using the Kontsevich integral representation, we are motivated to encode an MZV as a string of 0's and 1's, or rather as a string of y's and x's in the non-commutative polynomial ring $\mathbb{Q}\langle x, y \rangle$. This approach, explained below, is described in detail in [Hof05]. It provides a very elegant framework for stating important families of relations on MZV's.

With this encoding, we match the word $yx^{s_1 - 1} \cdots yx^{s_k - 1}$ with the multiple zeta value $\zeta(s_1, \ldots, s_k)$. Since $\zeta(s_1, \ldots, s_k)$ is convergent if and only if $s_k > 1$, this correspondence above lands in the vector subspace $\mathfrak{H}^0$ of *admissible words.*

Definition 1.1.17 (Subspace $\mathfrak{H}^0$)**.** The subspace of *admissible words* $\mathfrak{h}^0$ is the subspace of $\mathbb{Q}\langle x, y\rangle$, which is generated by words which start with a y, and end with an x.

We can then view ζ as a $\mathbb{Q}$-linear map $\zeta\colon \mathfrak{H}^0 \to \mathbb{R}$, sending $yx^{s_1-1}\cdots yx^{s_k-1}$ to the numerical value $\zeta(s_1, \ldots, s_k)$.

1.1.4.1 Duality of MZV's

Define the *anti*-automorphism $\tau\colon \mathbb{Q}\langle x, y\rangle \to \mathbb{Q}\langle x, y\rangle$ by $\tau(x) = y$, and $\tau(y) = x$. Then we have the following theorem.

Theorem 1.1.18 (Duality, Section 9 of [Zag94])**.** *Let $w \in \mathfrak{H}^0$ be any admissible word. Then*

$$\zeta(w) = \zeta(\tau(w)) \,.$$

Proof. This theorem is essentially proven by considering the integral representation. Let the admissible word $w = yx^{s_1-1}\cdots yx^{s_k-1}$. We have

$$\zeta(w) = (-1)^k I(0; 1, \{0\}^{s_1-1}, \ldots, 1, \{0\}^{s_k-1}; 1) \,.$$

Then apply the change of variables $t' = 1 - t$ in the iterated integral, to arrive at

$$= (-1)^k I(1; 0, \{1\}^{s_1-1}, \ldots, 0, \{1\}^{s_k-1}; 0) \,.$$

Now apply the reversal of paths property from Property 1.1.13 to get

$$= (-1)^k (-1)^{2+s_1+\cdots+s_k} I(0; \{1\}^{s_k-1}, 0, \ldots, \{1\}^{s_1}, 0; 1) \,.$$

However, this last integral has depth $(s_k - 1) + \cdots + (s_1 - 1) = s_1 + \cdots + s_k - k$. We can recognise the encoded word as $\tau(w)$, since the word has been reversed and we have interchanged $0 \leftrightarrow 1$. So this is

$$\begin{aligned} &= (-1)^k (-1)^{2+s_1+\cdots+s_k} (-1)^{s_1+\cdots+s_k-k} \zeta(\tau(w)) \\ &= \zeta(\tau(w)) \,, \end{aligned}$$

as claimed. □

From this theorem we get the promised one line proof of Euler's $\zeta(3) = \zeta(1, 2)$ result, Proposition 1.1.7. Consider $\zeta(3)$. This is encoded by the word $w = yx^2$. But $\tau(w) = y^2x$, which encodes $\zeta(1, 2)$, so we obtain $\zeta(3) = \zeta(1, 2)$ by the Duality theorem (Theorem 1.1.18).

Remark 1.1.19 (Duality of iterated integrals)**.** A restatement of the Duality theorem in terms of iterated integrals follows by applying the reversal of paths property, and the functoriality property under $t \mapsto 1 - t$ from Property 1.1.13. We have

$$I(0; a_1, \ldots, a_n; 1) = (-1)^n I(1; a_n, \ldots, a_1; 0) = (-1)^n I(0; 1 - a_n, \ldots, 1 - a_1; 1)$$

1.1.4.2 Shuffle product of MZV's

We know from the shuffle product property of iterated integrals in Property 1.1.13 that two iterated integrals with the same limits can be multiplied using the shuffle product. Since the integral representation of an MZV always has lower limit 0 and upper limit 1, we can multiply MZV's by multiplying their iterated integral representations.

The shuffle product $\sqcup\!\sqcup$ endows $(\mathbb{Q}\langle x, y\rangle, \sqcup\!\sqcup)$ with the structure of a commutative algebra. Since iterated integrals multiply with the shuffle product, we find that ζ is a homomorphism

$$\zeta\colon (\mathbb{Q}\langle x, y\rangle, \sqcup\!\sqcup) \to (\mathbb{R}, \,\cdot\,)\,.$$

More explicitly, this means that for any two words w_1 and w_2 in $\mathfrak{H}^0$, we have

$$\zeta(w_1)\zeta(w_2) = \zeta(w_1 \sqcup\!\sqcup\, w_2)\,.$$

Example 1.1.20. We can multiply out $\zeta(2)\zeta(2)$ using the shuffle product. We have that $\zeta(2)$ is encoded by $w = yx$. We get that

$$yx \sqcup\!\sqcup\, yx = 2 \cdot yxyx + 4 \cdot yyxx\,.$$

So

$$\zeta(2)\zeta(2) = \zeta(2 \cdot yxyx + 4 \cdot yyxx) = 2\zeta(2, 2) + 4\zeta(1, 3)\,.$$

1.1.4.3 Stuffle product of MZV's

Alternatively, we can multiply MZV's by multiplying their series representations. The product of two such series can be written as a sum of other MZV-type series, where the indices of summation are taken in all possible ways compatible with the original indices.

Rehashing the motivation for defining an MZV, we have the following example.

Example 1.1.21. Consider multiplying the series for $\zeta(2)$ with itself. We obtain

$$\zeta(2)\zeta(2) = \sum_{n>0} \frac{1}{n^2} \sum_{m>0} \frac{1}{m^2}\,.$$

By splitting up the summation region $\mathbb{Z}_{>0} \times \mathbb{Z}_{>0}$ into an upper triangle region, a lower triangular region, and a diagonal region, we obtain

$$\begin{aligned}
&= \sum_{n>m>0} \frac{1}{m^2 n^2} + \sum_{m>n>0} \frac{1}{n^2 m^2} + \sum_{n=m>0} \frac{1}{n^2 m^2} \\
&= \zeta(2, 2) + \zeta(2, 2) + \zeta(4) \\
&= 2\zeta(2, 2) + \zeta(4)\,.
\end{aligned}$$

This example generalises, and the associated multiplication is reflected in the *stuffle product* $*$ on $\mathbb{Q}\langle x, y\rangle$. For further details see [Hof92].

Definition 1.1.22 (Stuffle product)**.** The *stuffle product* $*$ on $\mathbb{Q}\langle x, y\rangle$ is defined recursively as follows.

i) For any word w, we have $1 * w = w * 1 = w$, where 1 is the empty word,

ii) For any word w and any integer $n \geq 1$, we have

$$x^n * w = w * x^n = wx^n \,,$$

iii) For any words w_1, w_2 and integers $p, q \geq 0$, we have

$$yx^p w_1 * yx^q w_2 = yx^p(w_1 * yx^q w_2) + yx^q(yx^p w_1 * w_2) + yx^{p+q+1}(w_1 * w_2)\,.$$

The stuffle product has a better interpretation on the MZV arguments themselves, rather than the xy-encoding strings. This interpretation can be obtained from the third part of Definition 1.1.22, namely: the MZV arguments are shuffled in all possible ways (coming from the first two terms), and two arguments can be *stuffed* into the same slot (coming from the third term, and alternatively just called 'extra *stuff*').

This endows $(\mathbb{Q}\langle x, y\rangle, *)$ with a different commutative algebra structure. Since the MZV series multiply with the $*$-product we find that ζ is a homomorphism

$$\zeta\colon (\mathbb{Q}\langle x, y\rangle, *) \to (\mathbb{R}, \,\cdot\,)\,.$$

More explicitly, this means for any two words w_1 and w_2 in $\mathfrak{H}^0$, we have

$$\zeta(w_1)\zeta(w_2) = \zeta(w_1 * w_2)\,.$$

1.1.4.4 (Regularised or extended) double shuffle on MZV's

We have two distinct ways of multiplying MZV's, so they demand to be compared. By expanding out a product of MZV's in the two different ways, the difference between both sides will be 0. This gives us *linear* relations between MZV's.

Example 1.1.23. In Example 1.1.20 we have an expression for $\zeta(2)\zeta(2)$ using the shuffle product. And in Example 1.1.21 we have an expansion for $\zeta(2)\zeta(2)$ using the stuffle product. Comparing the two leads to

$$2\zeta(2,2) + \zeta(4) \overset{\text{stuffle}}{=} \zeta(2)\zeta(2) \overset{\text{shuffle}}{=} 2\zeta(2,2) + 4\zeta(1,3)\,.$$

The difference between the left and right hand sides gives the identity

$$4\zeta(1,3) = \zeta(4)\,.$$

Remark 1.1.24. This identity (after evaluating $\zeta(4)$) is in fact a special case of the Zagier-Broadhurst identity that will form part of the background to Chapter 2.

Identity 1.1.25 (Double shuffle)**.** *For any $w_1, w_2 \in \mathfrak{H}^0$, the following standard family of linear relations on MZV's holds:*

$$\zeta(w_1 * w_2 - w_1 \sqcup\!\sqcup\, w_2) = 0\,.$$

It is known that the relations in Identity 1.1.25 are insufficient for generating *all* linear relations between MZV's. For example, the minimum possible weight of a double shuffle relation is 4, coming from $\zeta(2) \sqcup\!\sqcup\, \zeta(2) - \zeta(2) * \zeta(2)$, so the weight 3 result $\zeta(1,2) = \zeta(3)$ cannot arise. However, we can fix things by allowing a formal symbol $\zeta(1)$ for the divergent MZV, and extending the map ζ to certain non-admissible words. Comparing shuffle and stuffle leads to all divergent terms (formally) cancelling, and new linear relations appearing.

Identity 1.1.26 (Extended double shuffle)**.** *For any $w_1 \in \mathfrak{H}^1 \coloneqq \mathbb{Q}1 + y\mathbb{Q}\langle x, y\rangle$ and $w_2 \in \mathfrak{H}^0$, the following standard family of linear relations on MZV's holds:*

$$\zeta(w_1 * w_2 - w_1 \sqcup\!\sqcup\, w_2) = 0\,.$$

Here $\mathfrak{H}^1 \coloneqq \mathbb{Q}1 + y\mathbb{Q}\langle x, y\rangle$ corresponds to the inclusion of words not ending in x. Equivalently $\mathfrak{H}^1$ describes divergent MZV's $\zeta(n_1, n_2, \ldots, n_k)$ with $n_k = 1$.

Example 1.1.27. Consider expanding $\zeta(2)\zeta(1)$ using the stuffle and shuffle products. For the stuffle product we obtain

$$\zeta(2) * \zeta(1) = \zeta(yx * y) = \zeta(yyx + yxy + yxx) = \zeta(1,2) + \zeta(2,1) + \zeta(3)\,,$$

whereas for the shuffle product we obtain

$$\zeta(2) \sqcup\!\sqcup\, \zeta(1) = \zeta(yx \sqcup\!\sqcup\, y) = \zeta(2 \cdot yyx + yxy) = 2\zeta(1,2) + \zeta(2,1)\,.$$

The divergent term $\zeta(2,1)$ cancels when comparing the two equations, and leads to another proof of Euler's identity Proposition 1.1.7:

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

Remark 1.1.28. As it currently stands, Example 1.1.27 above is still only a formal proof. To be made rigorous one has to show that the formal cancellation of the divergent MZV's $\zeta(2,1)$ is actually allowed. This is proven rigorously in Sections 2 and 3 of [IKZ06], by defining certain regularisation procedures for the divergent MZV's, wherein the divergent $\zeta(1)$ is replaced by an indeterminate T. In Theorem 1 of [IKZ06], a comparison of these regularisation procedures gives relations between different MZV's. It is later shown in Theorem 2 of [IKZ06] that this comparison is equivalent to (among other things) the extended/regularised double shuffle relations in Identity 1.1.26.

Part of the procedure in [IKZ06] involves extracting the coefficient term of a polynomial in T (the formal symbol replacing $\zeta(1)$). This ends up setting $T = 0$, so one can interpret this as regularising $\zeta(1) \overset{\text{reg}}{=} 0$, to get finite values for the divergent MZV's. We will see this again when we discuss the shuffle regularisation of motivic iterated integrals in Section 1.2.3.1.

Conjecturally, all relations between MZV's come from this *regularised* comparision of shuffle and stuffle. Zudilin gives a precise version of this statement as follows.

Conjecture 1.1.29 (MZV relations, Conjecture 2 in [Zud03])**.** *The kernel of the ζ map, which describes all linear relations between MZV's, is given by*

$$\ker \zeta = \{ u ш v - u * v \mid u \in \mathfrak{H}^1, v \in \mathfrak{H}^0 \} \,,$$

where $\mathfrak{H}^1 := \mathbb{Q}1 + y\mathbb{Q}\langle x, y\rangle$ corresponds to the inclusion of words not ending in x. Equivalently $\mathfrak{H}^1$ describes divergent MZV's $\zeta(n_1, n_2, \ldots, n_k)$ with $n_k = 1$.

1.1.4.5 Examples of relations on MZV's

It is evident from the double-shuffle identities in Section 1.1.4.4 that MZV's should satisfy a large number of relations (something which is confirmed by the Dimension conjecture, in Section 1.1.5.3 below). Typically double-shuffle generates very messy and unstructured identities; one needs to combine carefully chosen double-shuffle relations to obtain more aesthetically pleasing identities. The purpose of this section is just to give a selection of these interesting or pretty identities, to make the theory a little concrete.

Identity 1.1.30. *Borwein, Bradley and Broadhurst [BBB97] use generating function methods to recover the following identity*

$$\zeta(\{2\}^n) = \frac{2(2\pi)^{2n}}{(2n+1)!} \left(\frac{1}{2}\right)^{2n+1} = \frac{\pi^{2n}}{(2n+1)!} \,,$$

which can also be established using a variant of Euler's method for evaluating $\zeta(2)$. More generally, they establish that $\zeta(\{2k\}^n) \in \pi^{2kn}\mathbb{Q} = \zeta(2kn)\mathbb{Q}$, with explicit expressions for small cases. The evaluations have a very particular form: a factor $\frac{2k(2\pi)^{2nk}}{(2kn+k)!}$ multiplied by a sum over certain algebraic numbers. For example,

$$\zeta(\{8\}^n) = \frac{8(2\pi)^{8n}}{(8n+4)!} \left(\left(1 + \frac{1}{\sqrt{2}}\right)^{4n+2} + \left(1 - \frac{1}{\sqrt{2}}\right)^{4n+2} \right) .$$

Identity 1.1.31 (Broadhurst-Zagier)**.** *The following identity was conjectured by Zagier [Zag94] on the basis of much numerical evidence. A proof was later provided by Broadhurst [BBBL01] using hypergeometric functions.*

$$\zeta(\{1,3\}^n) = \frac{2\pi^{4n}}{(4n+2)!} \,.$$

This identity is but the simplest example of a (largely) conjectural family of 'cyclic-insertion' identities that will be the focus of Chapter 2. The identity itself will be revisited in Section 2.1.1 when we sketch Broadhurst's proof, and fit the identity into a broader context.

Identity 1.1.32 (Gangl-Kaneko-Zagier, [GKZ06])**.** *The following identity on double zeta values $\zeta(a,b)$ is the first in an infinite family of identities which arise in connection to modular forms. There is a similar identity at weight k, whenever there is a non-trivial cusp form of weight k on Γ_1. The weight*

$k = 12$ *identity is*

$$28\zeta(3,9) + 150\zeta(5,7) + 168\zeta(7,5) = \frac{5197}{691}\zeta(12)\,.$$

Identity 1.1.33 (Cyclic derivations, Ohno)**.** *The following, very short, identity arises from applying Ohno's 'cyclic derivations' identity [HO03] to the word $w = (yx^2)^n$. One obtains*

$$\zeta(\{3\}^n, 4) = \zeta(1, 3, \{3\}^n) + \zeta(2, \{3\}^n, 2)\,.$$

1.1.5 Open questions about MZV's, and reasons for interest

With regard to multiple zeta values, one of the main areas of focus is the attempt to fully understand all the relations they satisfy. We have from Conjecture 1.1.29 a conjectural description of the space of all relations. This description entails plenty of further consequences, whose truth is still largely unknown.

1.1.5.1 Direct sum conjecture

All known relations between MZV's break up into relations between MZV's of the same weight. Conjecturally, all relations between MZV's are homogeneous, and so the vector space of MZV's is in fact weight graded. The Direct sum conjecture in [Fur03] essentially states:

Conjecture 1.1.34 (Direct sum conjecture)**.** *When regarded as a $\mathbb{Q}$-vector space, the space of MZV's is the direct sum of the subspaces $\mathcal{Z}_k$ of MZV's of weight k, so that all relations are homogeneous with respect to weight.*

From Conjecture 1.1.29, we have a conjectural description of the space of all MZV relations. It is clear from the statement of Conjecture 1.1.29 that the relations produced by comparing shuffle and stuffle are homogeneous.

1.1.5.2 Irrationality and transcendence

The irrationality, transcendence and linear independence properties of these numbers are still very mysterious. Thanks to Euler (Theorem 1.1.6) we know that $\zeta(2k) \in \pi^{2k}\mathbb{Q}$, so that all even zetas are irrational and $\mathbb{Q}$-algebraically dependent. Moreover, since π is transcendental, they are $\mathbb{Q}$-linearly independent.

The only other explicit result on irrationality of MZV's is due to Apéry, as recently as 1978, when he proved that $\zeta(3)$ is irrational [Apé79]. No one yet can even prove that $\zeta(5)$ is irrational, and aside from some curious non-explicit results like 'one of $\zeta(5), \zeta(7), \zeta(9)$ and $\zeta(11)$ is irrational', and 'infinitely many $\zeta(\text{odd})$ are irrational' [Riv00], little more is known. The question of proving $\zeta(5)$ and $\zeta(3)$ are even $\mathbb{Q}$-linearly independent, i.e. $\zeta(5)/\zeta(3)$ is irrational, seems hopelessly out of reach.

Morally, we do know what happens. We expect the following.

Conjecture 1.1.35 (Algebraic independence conjecture, Conjecture 1 in [Zud03])**.** *The numbers*

$$\pi, \zeta(3), \zeta(5), \zeta(7), \zeta(9), \ldots ,$$

are algebraically independent over $\mathbb{Q}$*.*

Moreover, as indicated above, no-one since Euler has been able to reduce $\zeta(3,5)$ to a polynomial in Riemann zeta values $\zeta(n)$. So in fact, we even expect

$$\zeta(3,5), \pi, \zeta(3), \zeta(5), \zeta(7), \zeta(9), \ldots ,$$

to be algebraically independent over $\mathbb{Q}$.

1.1.5.3 Dimension and basis conjectures

Following extensive numerical computations, searching for linear relations between MZV's, Zagier found numerically that the dimension of the space $\mathcal{Z}_k$ of MZV's of weight k is given by:

k	2	3	4	5	6	7	8	9	10	11	12
$\dim_{\mathbb{Q}} \mathcal{Z}_k$	1	1	1	2	2	3	4	5	7	9	12

This leads to the general conjecture in Section 9 of [Zag94] that $\dim_{\mathbb{Q}} \mathcal{Z}_k$ is given by the coefficient of x^k in the expansion of $\frac{1}{1-x^2-x^3}$, or equivalently by d_k, where d_k is defined by the recurrence relation:

$$\begin{cases} d_k = d_{k-2} + d_{k-3} \text{ with,} \\ d_2 = d_3 = d_4 = 1 \end{cases}$$

Conjecture 1.1.36 (Dimension conjecture, in Section 9 of [Zag94])**.** *The dimension of the space* $\mathcal{Z}_k$ *of MZV's of weight* k *is given by* d_k*, satisfying the recurrence* $d_k = d_{k-2} + d_{k-3}$ *with initial conditions* $d_2 = d_3 = d_4 = 1$*.*

This recurrence relating weight k MZV's to weight $k-2$ and weight $k-3$ in turn lead Hoffman to propose a candidate basis for the space $\mathcal{Z}_k$ might be given by $\zeta(w)$, where the word w is of weight k and satisfies $w \in \{2,3\}^\times$. That is, a basis might consist of zetas where the arguments are 2's and 3's only.

Conjecture 1.1.37 (Basis conjecture, Conjecture C in [Hof97].)**.** *A basis for the space* $\mathcal{Z}_k$ *is given by the Hoffman elements* $\zeta(n_1, \ldots, n_r)$*, where* $n_1, \ldots, n_r \in \{2,3\}$*, with weight* k*.*

It has since been proved, by various authors such as Goncharov [Gon02], Terasoma [Ter02] and Brown [Bro12a], that the upper bound $\dim_{\mathbb{Q}} \mathcal{Z}_k \leq d_k$ indeed holds. It is also known from Brown's work with motivic MZV's that the Hoffman elements, $\zeta(w)$ with $w \in \{\, 2,3 \,\}^\times$, do *span* the space of MZV's. Later, we can sketch some ideas from one proof of this which uses Brown's motivic MZV's, to be introduced below.

The reverse inequality is *much* harder to tackle. We don't even have a single proven instance where $\dim_{\mathbb{Q}} \mathcal{Z}_k > 1$. Nobody seriously entertains the notion that $\dim_{\mathbb{Q}} \mathcal{Z}_k = 1$, for $k \geq 5$, but for all we know the MZV's of weight k are all rational multiples of $\zeta(k)$, with immensely complicated rational factors we haven't identified yet.

1.2 Motivic MZV's

Motivic MZV's provide a way to study MZV's from a purely algebraic point of view, free from the analytic 'fiddleyness' that plagues the real-valued MZV's. Goncharov [Gon05, end of Section 1.2] goes as far as to claim that in his opinion "...an understanding of the transcendental aspects of the iterated integrals is impossible without investigation of the corresponding motivic objects".

Goncharov provides a construction of motivic iterated integrals. These motivic iterated integrals have a richer algebraic structure than the classical iterated integrals, in that form a Hopf algebra with coproduct Δ. By analogy with the Kontsevich integral representation of MZV's, Goncharov can then define motivic MZV's and make use of this Hopf algebra structure to study motivic MZV's. Unfortunately Goncharov's motivic MZV's are not completely satisfactory because his $\zeta^{\mathcal{M}}(2)$ element is necessarily 0. Brown's motivic MZV framework provides a refinement to this, further lifting the Hopf algebra of iterated integrals to a comodule where $\zeta^{\mathfrak{m}}(2) \neq 0$. The exact details of Gonchaov's motivic iterated integral construction, and the further refinements for Brown's motivic MZV framework, are not essential to the rest of this thesis, so we will provide only an overview of the construction.

The most important aspects of the motivic MZV framework for us are the combinatorial tools (namely the derivations D_r giving the infinitesimal coproduct, and Brown's theorem characterising $\ker D_{<N}$) which make it possible for us to algorithmically decompose motivic MZV's.

1.2.1 Goncharov's Hopf algebra of motivic iterated integrals

After fixing an embedding $\overline{\mathbb{Q}} \hookrightarrow \mathbb{C}$, Goncharov [Gon05] shows how the iterated integrals $I(x_0; x_1, \ldots, x_n; x_{n+1})$, defined in Section 1.1.3 above, can be upgraded to *framed mixed Tate motives over* $\overline{\mathbb{Q}}$, at least when the parameters x_i are algebraic numbers. This procedure gives us a *motivic iterated integral*:

$$I^{\mathcal{M}}(x_0; x_1, \ldots, x_n; x_{n+1}) \in \mathcal{A}_n(\overline{\mathbb{Q}})$$

that by definition lies in a commutative, graded Hopf algebra $\mathcal{A}_\bullet(\overline{\mathbb{Q}})$.

Assuming the parameters x_i are algebraic numbers, there are only finitely many, so one can suppose they lie in some number field F, rather than just in $\overline{\mathbb{Q}}$. Then the graded, commutative Hopf algebra $\mathcal{A}_\bullet(F)$ is the (unipotent quotient of the) fundamental de Rham Hopf algebra of the abelian category $\mathcal{MT}(F)$ of *mixed Tate motives over* F.

Since the motivic iterated integrals lie in a Hopf algebra, they admit a coproduct Δ. This is a genuinely new algebraic structure on iterated integrals; it is completely invisible at the level of numbers. Goncharov [Gon05] proves that the coproduct is as follows.

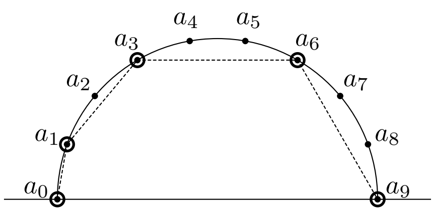
Theorem 1.2.1 (Goncharov, Theorem 1.2 in [Gon05])**.** *The coproduct on the Hopf algebra of motivic iterated integrals is given by the formula*

$$\Delta I^{\mathcal{M}}(a_0; a_1, \dots, a_n; a_{n+1}) =$$
$$\sum_{0=i_0<i_1<\ldots<i_k<i_{k+1}=n+1} I^{\mathcal{M}}(a_0; a_{i_1}, \dots, a_{i_k}; a_{n+1}) \otimes \prod_{p=0}^{k} I^{\mathcal{M}}(a_{i_p}; a_{i_p+1}, \dots, a_{i_{p+1}-1}; a_{i_{p+1}})$$

Remark 1.2.2. This formula has an elegant interpretation in terms of cutting off segments of a semicircular polygon. For example, the term:

$$I^{\mathcal{M}}(a_0; a_1, a_3, a_6; a_9) \otimes I^{\mathcal{M}}(a_0; a_1) I^{\mathcal{M}}(a_1; a_2; a_3) I^{\mathcal{M}}(a_3; a_4, a_5; a_6) I^{\mathcal{M}}(a_6; a_7, a_8; a_9)$$

in the coproduct $\Delta I^{\mathcal{M}}(a_0; a_1, \dots, a_8; a_9)$ corresponds to cutting off the indicated segments from the semicircular polygon below:



The other terms arise from taking all other possible choices of segments.

There is a canonical surjective homomorphism:

$$p_\sigma \colon \mathcal{A}_\bullet(F) \to \mathcal{P}^\sigma_\bullet(F)$$
$$I^{\mathcal{M}}(a_0; a_1, \dots, a_n; a_{n+1}) \mapsto \overline{I}(\sigma(a_0); \sigma(a_1), \dots, \sigma(a_n); \sigma(a_{n+1}))$$

that realises a motivic iterated integral by the projection of its classical counterpart to the associated graded $\mathcal{P}^\sigma_\bullet(F)$ of the filtered algebra $\mathcal{P}^\sigma(F)$ of periods of mixed Tate motives over F. (Here $\sigma \colon F \hookrightarrow \mathbb{C}$ is an embedding of F into $\mathbb{C}$.) Roughly, this means that any relations satisfied on the motivic level also hold on the level of classical integrals, modulo integrals of lower weight.

Conjecturally this map p_σ should in fact define an isomorphism from the $\mathbb{Q}$-vector space of motivic iterated integrals to the $\mathbb{Q}$-vector space of periods of mixed Tate motives over F. Whether or not this is true, as a purely algebraic lifting of iterated integrals to motivic iterated integrals, we gain the structure of a Hopf algebra, and eliminate the transcendence problems that plague the classical iterated integrals. We can therefore use these motivic iterated integrals to gain new insights into the classical iterated integrals.

1.2.2 Goncharov's motivic MZV's

With the Kontsevich integral representation of multiple zeta values, we can make the following definition to obtain Goncharov's *motivic* MZV's.

Definition 1.2.3. Goncharov's motivic multiple zeta value $\zeta^{\mathcal{M}}(s_1, \ldots, s_k)$ is defined by

$$\zeta^{\mathcal{M}}(s_1, \ldots, s_k) = (-1)^k I^{\mathcal{M}}(0; 1, \{0\}^{s_1-1}, \ldots, 1, \{0\}^{s_k-1}; 1)\,.$$

With this definition, Goncharov notes that $\zeta^{\mathcal{M}}(2k) = 0$ because $(2\pi \mathrm{i})^{-2k}\zeta(2k) \in \mathbb{Q}$ and $\mathcal{A} = \mathcal{O}(\mathcal{U}^{\mathcal{M}})$, the ring of regular functions on the unipotent part of the motivic Galois group. However, $\zeta^{\mathcal{M}}(2k+1) \neq 0$ in this setting, and here we get to see the first success of the motivic viewpoint in eliminating the analytic difficulties of MZV's.

Proposition 1.2.4 (Goncharov, [Gon05])**.** *Although no-one can prove yet that the numbers $\zeta(2k+1)$ are linearly independent over $\mathbb{Q}$, we have that the motivic elements*

$$\zeta^{\mathcal{M}}(2k+1) \in \mathcal{A}_{2k+1}(\mathbb{Q})$$

are linearly independent over $\mathbb{Q}$.

Proof. The elements belong to components of different degrees in $\mathcal{A}_\bullet(\mathbb{Q})$. Therefore they must be linearly independent over $\mathbb{Q}$. □

In fact we can prove even more than this. Not only are the elements $\zeta^{\mathcal{M}}(2k+1)$ linearly independent over $\mathbb{Q}$, they are in fact algebraically independent over $\mathbb{Q}$, as expected from Conjecture 1.1.35.

Theorem 1.2.5. *The odd motivic multiple zeta values $\zeta^{\mathcal{M}}(3), \zeta^{\mathcal{M}}(5), \zeta^{\mathcal{M}}(7), \ldots, \zeta^{\mathcal{M}}(2n+1), \ldots$ are algebraically independent over $\mathbb{Q}$.*

Proof. We will prove this by a induction on the size of the purported algebraically dependent set.

Firstly we observe that the odd motivic MZV $\zeta^{\mathcal{M}}(2n+1)$ is transcendental over $\mathbb{Q}$. That is, $\zeta^{\mathcal{M}}(2n+1)$ is not a root of any non-zero polynomial $f(x) \in \mathbb{Q}[x]$. This is an easy observation because of the weight grading of motivic MZV's. Suppose that $f(x) = \sum_{i=0}^k \alpha_i x^i$ is a non-zero polynomial of degree k which has $\zeta^{\mathcal{M}}(2n+1)$ as a root. Then we have $a_k \neq 0$ and $a_i = 0$ for $i < k$ because of the weight grading. So weight $(2n+1)k$ part of this relation is only $\alpha_k \zeta^{\mathcal{M}}(2n+1)^k = 0$. Since $\zeta^{\mathcal{M}}(2n+1) \neq 0$, we conclude that $\alpha_k = 0$, contradicting our definition of f.

We thus have that any size 1 set of odd motivic MZV's is algebraically independent over $\mathbb{Q}$. Suppose now that $S = \left\{ \zeta^{\mathcal{M}}(a_1), \ldots, \zeta^{\mathcal{M}}(a_\ell) \right\}$ is a set of ℓ odd motivic MZV's, and that any set of size $\leq \ell - 1$ other odd motivic MZV's is algebraically independent over $\mathbb{Q}$. We will prove that S is also algebraically independent over $\mathbb{Q}$.

Suppose to the contrary, that S is algebraically dependent over $\mathbb{Q}$. Without loss of generality, assume that $a_1 < a_2 < \cdots < a_\ell$. Let

$$f(x_1, \ldots, x_\ell) = \sum_{i_1,\ldots,i_\ell} \alpha_{i_1,\ldots,i_\ell} x_1^{i_1} \cdots x_\ell^{i_\ell}$$

be the minimal polynomial witnessing this algebraic dependence. Here the sum runs over $i_1, \ldots, i_\ell \geq 0$ with $\sum a_j i_j = N$, for some fixed weight N, and minimal means in terms of the total degree. With this polynomial we have $f(\zeta^{\mathcal{M}}(a_1), \ldots, \zeta^{\mathcal{M}}(a_\ell)) = 0$. Now apply the coproduct, and look at the weight $(a_1, N - a_1)$ component. In the coproduct, $\zeta^{\mathcal{M}}(a_1) \mapsto 1 \otimes \zeta^{\mathcal{M}}(a_1) + \zeta^{\mathcal{M}}(a_1) \otimes 1$, so the only way to obtain $\zeta^{\mathcal{M}}(a_1) \otimes \cdots$ is via the $\zeta^{\mathcal{M}}(a_1) \otimes \zeta^{\mathcal{M}}(a_1)^{i_1 - 1}$ term from $\Delta\zeta^{\mathcal{M}}(a_1)^{i_1}$, and the $1 \otimes \zeta^{\mathcal{M}}(a_k)^{i_k}$ terms from each $\Delta\zeta^{\mathcal{M}}(a_k)^{i_k}$. We get that the weight $(a_1, N - a_1)$ component is

$$\zeta^{\mathcal{M}}(a_1) \otimes \left(\sum_{i_1,\ldots,i_\ell} \alpha_{i_1,\ldots,i_\ell} \binom{i_1}{1} \zeta^{\mathcal{M}}(a_1)^{i_1 - 1} \zeta^{\mathcal{M}}(a_2)^{i_2} \cdots \zeta^{\mathcal{M}}(a_\ell)^{i_\ell} \right) .$$

Here the sum runs over $i_1 \geq 1$ and $i_2, \ldots, i_\ell$ with $\sum a_j i_j = N$.

Since the coproduct $\Delta f(\zeta^{\mathcal{M}}(a_1), \ldots, \zeta^{\mathcal{M}}(a_\ell)) = \Delta 0 = 0$, we must have that this $(a_1, N - a_1)$ degree component already vanishes. Since $\zeta^{\mathcal{M}}(a_1) \neq 0$, we obtain

$$\sum_{i'_1,\ldots,i'_\ell} \alpha_{i'_1+1, i'_2, \ldots, i'_\ell} (i'_1 + 1) \zeta^{\mathcal{M}}(a_1)^{i'_1} \zeta^{\mathcal{M}}(a_2)^{i'_2} \cdots \zeta^{\mathcal{M}}(a_\ell)^{i'_\ell} = 0$$

after changing variables $i'_1 = i'_1 - 1$, and otherwise $i'_j = i_j$. Here the sum runs over all $i'_1, \ldots, i'_\ell \geq 0$ with $\sum a_j i_j = N - a_1$.

We see that this combination is a strictly lower degree polynomial under which the algebraic dependence of $\zeta^{\mathcal{M}}(a_1), \ldots, \zeta^{\mathcal{M}}(a_\ell)$ is witnessed. This is not possible by out assumption that f is the minimal such polynomial, so we conclude that $\alpha_{i'_1+1, i'_2, \ldots, i'_\ell}(i'_1 + 1) = 0$. Since $i'_1 + 1 \geq 0 + 1 = 1$, we find that $\alpha_{i'_1+1, i'_2, \ldots, i'_\ell} = 0$, for $i'_j \geq 0$.

Plugging this information about α back into the polynomial f, we obtain

$$f(x_1, \ldots, x_\ell) = \sum_{i_2,\ldots,i_\ell} \alpha_{0, i_2, \ldots, i_\ell} x_2^{i_2} \cdots x_\ell^{i_\ell} =: \widetilde{f}(x_2, \ldots, x_\ell)$$

is independent of x_1. Since $S' = \left\{ \zeta^{\mathcal{M}}(a_2), \ldots, \zeta^{\mathcal{M}}(a_\ell) \right\}$ is algebraically independent over $\mathbb{Q}$ by assumption (being a set of size $\ell - 1$), we must have that $\alpha_{0, i_2, \ldots, i_\ell} = 0$ also, to ensure that $\widetilde{f}$ is identically 0.

This now shows that f itself is identically 0. So the polynomial witnessing the algebraic dependence of $S = \left\{ \zeta^{\mathcal{M}}(a_1), \ldots, \zeta^{\mathcal{M}}(a_\ell) \right\}$ is identically 0. This is a contradiction since such a polynomial must be non-zero. Hence the set S is in fact algebraically independent over $\mathbb{Q}$.

Since we established directly that any set of size 1 is algebraically independent over $\mathbb{Q}$, we obtain by induction a proof that any finite set S of odd motivic MZV's is algebraically independent over $\mathbb{Q}$. This proves the claim about the $\mathbb{Q}$-algebraic independence of $\zeta^{\mathcal{M}}(3), \zeta^{\mathcal{M}}(5), \zeta^{\mathcal{M}}(7), \ldots, \zeta^{\mathcal{M}}(2k + 1), \ldots$. $\square$

In the same paper [Gon05], Goncharov gives an application of this motivic iterated integral framework, and motivic multiple zeta value framework, to the detailed study of the motivic double zeta values.

One application is to show that $\zeta^{\mathcal{M}}(3,5)$ is irreducible.

Proposition 1.2.6 (Goncharov, [Gon05])**.** *The motivic MZV $\zeta^{\mathcal{M}}(3,5)$ is irreducible, so cannot be expressed as a polynomial in Riemann zeta values $\zeta^{\mathcal{M}}(n)$.*

Sketch proof: Make use of the restricted coproduct Δ', defined by $\Delta'(x) = \Delta(x) - 1 \otimes x - x \otimes 1$. One has that if $\Delta'(x) = \Delta'(y) = 0$, then $\Delta'(xy) = x \otimes y + y \otimes x$.

One computes that

$$\Delta'(\zeta^{\mathcal{M}}(3,5)) = -5 \cdot \zeta^{\mathcal{M}}(3) \otimes \zeta^{\mathcal{M}}(5) \,.$$

Since $\zeta^{\mathcal{M}}(2n+1) \neq 0$, this shows that $\zeta^{\mathcal{M}}(3,5) \neq 0$ also.

Moreover if $\zeta^{\mathcal{M}}(3,5)$ were a (sum of) products of Riemann zeta values, we could antisymmetrise and the result would vanish by the computation $\Delta'(xy)$ above.

But antisymmetrising $\Delta'(\zeta^{\mathcal{M}}(3,5)) = -5 \cdot \zeta^{\mathcal{M}}(3) \otimes \zeta^{\mathcal{M}}(5)$ gives $-5 \cdot \zeta^{\mathcal{M}}(3) \wedge \zeta^{\mathcal{M}}(5) \neq 0$. This proves that $\zeta^{\mathcal{M}}(3,5)$ cannot be expressed as a polynomial in Riemann zeta values, so is irreducible. □

A second application Goncharov gives is to prove that the motivic double shuffle relations suffice to generate all relations on motivic double zeta values.

Theorem 1.2.7 (Goncharov, Theorem 6.5 in [Gon05])**.** *Consider the generating series $\overline{\zeta}^{\mathcal{M}}(t_0, t_1, t_2) \coloneqq \overline{\zeta}^{\mathcal{M}}(t_1, t_2)$, where $t_0 + t_1 + t_2 = 0$, and $\overline{\zeta}^{\mathcal{M}}$ is the projection of $\zeta^{\mathcal{M}}$ modulo products and depth 1 terms. We have*

i) The generating series $\overline{\zeta}^{\mathcal{M}}(t_0, t_1, t_2)$ satisfies the dihedral symmetry relations

$$\overline{\zeta}^{\mathcal{M}}(t_0, t_1, t_2) = \overline{\zeta}^{\mathcal{M}}(t_1, t_2, t_0) = -\overline{\zeta}^{\mathcal{M}}(t_0, t_2, t_1) = \overline{\zeta}^{\mathcal{M}}(-t_0, -t_1, -t_2) \,,$$

which are the motivic analogue of the (regularised) double shuffle relations.

ii) And there are no other relations between the coefficients of the generating series $\overline{\zeta}^{\mathcal{M}}(t_0, t_1, t_2)$.

Goncharov's motivic iterated integrals, and motivic MZV's, do provide new insight into the structure of real MZV's. However, they are not a perfect tool for studying real MZV's: the motivic element $\zeta^{\mathcal{M}}(2)$ vanishes, so we miss out on this part of the story. Because $\zeta^{\mathcal{M}}(2) = 0$, there is no period map down to $\mathbb{C}$, so we cannot compare numerically with the real valued classical MZV relations. Brown's motivic MZV framework plugs this gap.

1.2.3 Brown's motivic MZV's

In [Bro12a], Brown shows how Goncharov's motivic iterated integrals can be further lifted in such a way that $\zeta^{\mathfrak{m}}(2)$ is non-zero. (Brown uses the notation $\mathfrak{m}$ for his motivic elements.)

For parameters $a_i \in \{ 0, 1 \}$, the motives corresponding to Goncharov's motivic iterated integrals $I^{\mathcal{M}}(a_0; a_1, \ldots, a_n; a_{n+1})$ are unramified over $\mathbb{Z}$, so they lie in $\mathcal{A}^{\mathcal{MT}} := \mathcal{A}_\bullet(\mathbb{Z})$. We can then introduce a trivial comodule over $\mathcal{A}^{\mathcal{MT}}$, defined by

$$\mathcal{H}^{\mathcal{MT}_+} := \mathcal{A}^{\mathcal{MT}} \otimes_{\mathbb{Q}} \mathbb{Q}[f_2] \,,$$

where f_2 is taken to be of degree 2. This f_2 will correspond to the non-zero lifting of Goncharov's $\zeta^{\mathcal{M}}(2)$.

In Theorem 3.5 of [Bro12b] Brown then proves that there is a Hopf subalgebra $\mathcal{A}$ of $\mathcal{A}^{\mathcal{MT}}$, and a graded comodule $\mathcal{H} = \mathcal{H}_\bullet$ over $\mathcal{A}$, satisfying the following properties. (See section 2 of [Bro12a], or the summary in Theorem 3.5 of [Bro12b])

- It is spanned by the motivic iterated integrals

  $$I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) \in \mathcal{H}_n \,,$$

  with $a_i \in \{ 0, 1 \}$, satisfying the standard properties of iterated integrals given in Section 1.1.3.

- There is a period map

  $$\mathrm{per}\colon \mathcal{H} \to \mathbb{R} \tag{1.2.1}$$
  $$I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) \mapsto I(a_0; a_1, \ldots; a_n; a_{n+1}) \,, \tag{1.2.2}$$

  which is a ring homomorphism. This means that motivic relations descend exactly to relations on classical MZV's.

- There is a non-canonical isomorphism of Hopf algebra comodules

  $$\mathcal{H} \cong \mathcal{A} \otimes_{\mathbb{Q}} \mathbb{Q}[\zeta^{\mathfrak{m}}(2)] \,,$$

  and a non-canonical embedding of Hopf algebra comodules $\mathcal{H} \hookrightarrow \mathcal{H}^{\mathcal{MT}_+}$, which sends $\zeta^{\mathfrak{m}}(2) = -I^{\mathfrak{m}}(0; 1, 0; 1)$ to f_2. $\zeta^{\mathfrak{m}}(2)$ is non-zero in this incarnation.

Given Brown's motivic iterated integrals, we can make an analogous definition of a motivic multiple zeta value.

Definition 1.2.8. Brown's motivic multiple zeta value $\zeta^{\mathfrak{m}}(s_1, \ldots, s_k)$ is defined by

$$\zeta^{\mathcal{M}}(s_1, \ldots, s_k) = (-1)^k I^{\mathfrak{m}}(0; 1, \{0\}^{s_1 - 1}, \ldots, 1, \{0\}^{s_k - 1}; 1) \,.$$

1.2.3.1 Shuffle regularisation of (motivic) MZV's

When dealing with (motivic) MZV's, we obtain iterated integrals from $x_0 = 0$ to $x_{n+1} = 1$ which start with $x_1 = 1$ and end with $x_n = 1$, as in $I(0; 1, \ldots, 0; 1)$. In particular the corresponding real-valued integrals are always convergent. It will be convenient (indeed necessary) to expand the class of allowed integrals to include divergent integrals by assigning them a finite value in a precise way. This process of assigning a finite value to divergent integrals is known as regularisation.

The procedure for regularising iterated integrals is described by Brown, in Section 2.4 of [Bro12b] for the real-valued MZV's. A more explicit and precise procedure for doing this for motivic iterated integrals is given in Section 5.1 of [Bro12b], in the paragraph following the list of relations. This motivic procedure is equally applicable to the real-valued integrals.

After regularising the divergent integral $I^{\mathfrak{m}}(0;0;1) \overset{\text{reg}}{=} 0$, using property I1 [Theorem 3.5 in Bro12b], we can regularise any divergent integral with parameters $x_i \in \{ 0, 1 \}$ that starts $I^{\mathfrak{m}}(0;0,\ldots)$ by repeated application of the shuffle product formula. Any remaining divergences must be integrals that end $I^{\mathfrak{m}}(\ldots,1;1)$, which can be reduced to the previous case by duality.

Specifically, this regularisation is by way of relation R2 [Section 5.1 in Bro12b].

$$(-1)^k I^{\mathfrak{m}}(0;\{0\}^k,1,\{0\}^{n_1-1},\ldots,1,\{0\}^{n_r-1};1) = \sum_{i_1+\cdots+i_r=k} \binom{n_1-1+i_1}{i_1}\cdots\binom{n_r-1+i_r}{i_r} I^{\mathfrak{m}}(0;1,\{0\}^{n_1+i_1-1},\ldots,1,\{0\}^{n_r+i_r-1};1)\,, \tag{1.2.3}$$

to deal with divergences where the integral starts $I^{\mathfrak{m}}(0;0,\ldots)$. This is is proven by repeated application of the shuffle product identity

$$0 = I^{\mathfrak{m}}(0;0;1)I^{\mathfrak{m}}(0;w;1) = I^{\mathfrak{m}}(0;0 \sqcup\!\sqcup w;1)\,,$$

coupled with the result that $I^{\mathfrak{m}}(0;0;1) \overset{\text{reg}}{=} 0$. Divergences where the integral ends $I^{\mathfrak{m}}(\ldots,1;1)$, are dealt with by applying duality, to reduce to the above case.

Example 1.2.9. For example, to regularise $z = I(0;0,1,0,1,1;1)$, we first apply rule R2 to get

$$\begin{aligned} z &= I(0;\underbrace{0}_{k=1},\underbrace{1,0}_{n_1=2},\underbrace{1}_{n_2=1},\underbrace{1}_{n_3=1};1) \\ &= (-1)^1 \sum_{i_1+i_2+i_3=1} \binom{1+i_1}{i_1}\binom{0+i_2}{i_2}\binom{0+i_3}{i_3} I(0;1,\{0\}^{1+i_1},1,\{0\}^{0+i_2},1,\{0\}^{0+i_3};1) \\ &= -2I(0;1,0,0,1,1;1) - 1I(0;1,0,1,0,1;1) - 1I(0;1,0,1,1,0;1)\,. \end{aligned}$$

The third term is now okay. Apply duality to the first and second, to get

$$z = -2I(0;0,0,1,1,0;1) - 1I(0;0,1,0,1,0;1) - 1I(0;1,0,1,1,0;1)\,.$$

Now we can apply the rule R2 procedure to the first and second terms to obtain

$$\begin{aligned} z = &-2(I(0;1,0,0,1,0;1) + 2I(0;1,0,1,0,0;1) + 3I(0,1,1,0,0,0;1)) + \\ &-(-2I(0;1,0,0,1,0;1) - 2I(0;1,0,1,0,0;1)) + \\ &-I(0;1,0,1,1,0;1) \\ = &\ 2I(0;1,0,1,0,0,1) - I(0;1,0,1,1,0;1) + 6I(0;1,1,0,0,0;1)\,. \end{aligned}$$

At last, these integrals can be converted to MZV's, and we obtain

$$z = 2\zeta(2,3) + \zeta(2,1,2) + 6\zeta(1,4)$$

This regularisation procedure is closely related to the regularisation procedure mentioned in Remark 1.1.28, which is used in rigorously defining the extended double shuffle relations. There one regularises $\zeta(1) \overset{\text{reg}}{=} 0$. This is equivalent to regularising $I^{\mathfrak{m}}(0;0;1) \overset{\text{reg}}{=} 0$ here by duality. One can then reinterpret Example 1.1.27 in a perhaps more rigorous way.

Firstly, we compute the following regularisation of $\zeta(2,1)$. We have that $\zeta(2,1) = I(0;1,0,1;1) = -I(0;0,1,0;1)$ by duality. Then

$$\begin{aligned} I(0; \underbrace{0}_{k=0}, \overbrace{1,0}^{n_1=2}, 1) &= (-1)^k \sum_{i_1=1} \binom{n_1 - 1 + i_1}{i_1} I(0;1,\{0\}^{n_1-1+i_1};1) \\ &= -2I(0;1,0,0;1) \\ &= 2\zeta(3)\,, \end{aligned}$$

so that $\zeta(2,1) \overset{\text{reg}}{=} -2\zeta(3)$.

Example 1.2.10. Recall the computations from Example 1.1.27, where we established

$$\begin{aligned} \zeta(1) * \zeta(2) &= \zeta(2,1) + \zeta(1,2) + \zeta(3) \\ \zeta(1) ⧢ \zeta(2) &= \zeta(2,1) + 2\zeta(1,2)\,. \end{aligned}$$

Apply to this the regularisation $\zeta(2,1) \overset{\text{reg}}{=} -2\zeta(3)$ computed above, and we get

$$\begin{aligned} \zeta(1) * \zeta(2) &\overset{\text{reg}}{=} \zeta(1,2) - \zeta(3) \\ \zeta(1) ⧢ \zeta(2) &\overset{\text{reg}}{=} -2\zeta(3) + 2\zeta(1,2)\,. \end{aligned}$$

The comparison between regularised values is allowed by Theorem 2 of [IKZ06], and so we derive once again $\zeta(1,2) = \zeta(3)$.

1.2.3.2 'Levels' of motivic MZV's

In section 3.3 of [Bro12b], Brown explains how these motivic MZV's exist on a number of different levels. On the highest level we have the comodule $\mathcal{H}$, where $\zeta^{\mathfrak{m}}(2) \neq 0$.

Then we have the Hopf algebra

$$\mathcal{A} = \mathcal{H}/\zeta^{\mathfrak{m}}(2)\mathcal{H}\,,$$

in which $\zeta^{\mathfrak{m}}(2)$ is killed. Brown writes $\zeta^{\mathfrak{a}}$ for the image of $\zeta^{\mathfrak{m}}$ under the quotient map $\mathcal{H} \to \mathcal{A}$. The elements $\zeta^{\mathfrak{a}}(n_1, \ldots, n_r)$ are Goncharov's motivic MZV's, discussed in Section 1.2.2 above.

Finally have the Lie coalgebra

$$\mathcal{L} = \frac{\mathcal{A}_{>0}}{\mathcal{A}_{>0}\mathcal{A}_{>0}}\,,$$

of indecomposable elements in $\mathcal{A}$. This Lie coalgebra will play a role in the 'infinitesimal' version of the coaction to be introduced below. Brown denotes the image in $\mathcal{L}$ of an element $\zeta^{\mathfrak{m}}$ as $\zeta^{\mathfrak{L}}$.

The same notation is used for the image of a motivic iterated integral $I^{\mathfrak{m}}$ in $\mathcal{A}$, and in $\mathcal{L}$, namely $I^{\mathfrak{a}}$ and $I^{\mathfrak{L}}$ respectively.

This is summarised in equation 3.13 of [Bro12b], as follows

$$\begin{array}{ccccc} \mathcal{H} & \longrightarrow & \mathcal{A} & \longrightarrow & \mathcal{L} \\ \zeta^{\mathfrak{m}}(w) & \longmapsto & \zeta^{\mathfrak{a}}(w) & \longmapsto & \zeta^{\mathfrak{L}}(w) \\ I^{\mathfrak{m}}(w) & \longmapsto & I^{\mathfrak{a}}(w) & \longmapsto & I^{\mathfrak{L}}(w) \end{array}$$

1.2.3.3 Coaction, and the infinitesimal coaction

As discussed in Section 1.2.1, Goncharov [Gon05] showed how to compute the coproduct $\Delta\colon \mathcal{A}\otimes_{\mathbb{Q}}\mathcal{A} \to \mathcal{A}$ for his motivic iterated integrals $I^{\mathfrak{a}}(a_0; a_1, \ldots, a_n; a_{n+1}) = I^{\mathcal{M}}(a_0; a_1, \ldots, a_n; a_{n+1})$. By lifting $\mathcal{A}$ to the comodule $\mathcal{H}$, we now get a coaction $\Delta\colon \mathcal{H} \to \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}$.

In Theorem 2.4 of [Bro12a], Brown shows that the coaction for his motivic MZV's is given by the same formula as Goncharov's coproduct, up to swapping the factors:

Theorem 1.2.11 (Brown, Theorem 2.4 in [Bro12a])**.** *The coaction for the motivic multiple zeta values is given by the following formula*

$$\Delta I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) =$$
$$\sum_{0<i_0<i_1<\cdots<i_k<i_{k+1}=n+1} \left(\prod_{p=0}^{k} I^{\mathfrak{a}}(a_{i_p}; a_{i_p+1}, \ldots, a_{i_{p+1}-1}; a_{i_{p+1}}) \right) \otimes I^{\mathfrak{m}}(a_0; a_{i_1}, \ldots, a_{i_k}; a_{n+1}) \,.$$

In order to make explicit calculations with the coaction more tractable, Brown wants to consider an infinitesimal version of it which factors through a family of operators D_r. The coaction above involves an exponential number of terms, as the weight grows. But the infinitesimal coaction will only have a quadratic number of terms (each operator D_r has a linear number of terms, and there are a linear number of D_r operators as the weight grows).

In section 4 of [Bro12b], Brown shows how the infinitesimal coproduct factors through the family of operators D_r, for odd $r \geq 3$.

Definition 1.2.12 (Definition 4.4 in [Bro12b])**.** The operators D_r, for odd $r \geq 3$ are defined as the projection onto the Lie coalgebra of the weight $(r, N-r)$-graded part of the coaction. Namely

$$D_r\colon \mathcal{H}_N \xrightarrow{\Delta_{r,N-r}} \mathcal{A}_r \otimes_{\mathbb{Q}} \mathcal{H}_{N-r} \xrightarrow{\pi\otimes\mathrm{id}} \mathcal{L}_r \otimes_{\mathbb{Q}} \mathcal{H}_{N-r} \,.$$

Here $\mathcal{L}_r$ refers to the degree r component of the Lie coalgebra of indecomposables $\mathcal{L}$. Similarly $\Delta_{r,N-r}$ is the part of the coproduct which lands in the degree $(r, N-r)$ component of $\mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}$. Finally π is the quotient map

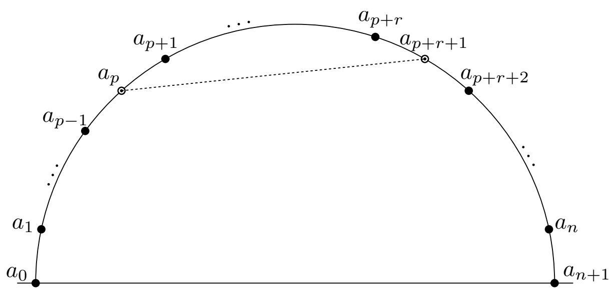
$$\pi\colon \mathcal{A}_{>0} \to \mathcal{L} \coloneqq \frac{\mathcal{A}_{>0}}{\mathcal{A}_{>0} \cdot \mathcal{A}_{>0}}\,.$$

From the computation of the coaction Δ above, Brown obtains the following computation of the action of D_r.

Proposition 1.2.13. *The operator D_r acts in the following way on the element $I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1})$.*

$$D_r I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1}) =$$
$$\sum_{p=0}^{n-r} I^{\mathfrak{L}}(a_p; a_{p+1}, \ldots, a_{p+r}; a_{p+r+1}) \otimes I^{\mathfrak{m}}(a_0; a_1, \ldots, a_p, a_{p+r+1}, \ldots, a_n; a_{n+1})\,.$$

Like Goncharov's coproduct, these derivations have an interpretation in terms of cutting segments out of a semicircular polygon. The operator D_r can be viewed as cutting off a segment with r points, from the semicircular polygon. By cutting off all such possible segments, we get D_r.



It is important to note that the boundary terms a_p and a_{p+r+1} appear in both the left- and right-hand factors of D_r, so they are part of both the main polygon, and the cut-off segment above.

It is convenient to give names to the left and right hand terms appearing above. Brown uses the relation between the formula for D_r, and the Connes-Kreimer coproduct for a certain class of graphs to make the following definitions.

Definition 1.2.14 (Subsequence, quotient sequence, trivial subsequence)**.** In the formula for $D_r I^{\mathfrak{m}}(a_0; a_1, \ldots, a_n; a_{n+1})$, we name the terms as follows:

- The sequence appearing on the left

  $$(a_p; a_{p+1}, \ldots, a_{p+r}; a_{p+r+1})$$

  is called the *subsequence*.

- The sequence appearing on the right

  $$(a_0; a_1, \ldots, a_p, a_{p+r}, \ldots, a_n; a_{n+1})$$

  is called the *quotient sequence*.

Notice that the subsequence for D_r contains r *interior* points, for a total of $r+2$ points.

If $a_p = a_{p+r+1}$ in the subsequence, we will call the subsequence *trivial*. This is because the integral $I^{\mathfrak{L}}(a_p; a_{p+1}, \ldots, a_{p+r}; a_{p+r+1}) = 0$ by the equal boundaries property in Property 1.1.13

Roughly, these operators D_r are used to decompose a motivic MZV into a chosen basis. The operator D_r extracts the coefficient of $\zeta^{\mathfrak{m}}(2k+1)$ as a polynomial in this basis. This forms part of an 'exact-numerical' algorithm to decompose an MZV, as explained in section 5 of [Bro12b].

The upshot of this algorithm, and the operators D_r, is the following theorem. This theorem gives us very combinatorial tools for producing and checking identities on MZV's. For many purposes, the tools themselves can be applied easily, without worrying about the motivic framework behind them.

Theorem 1.2.15 (Brown, Theorem 3.3 in [Bro12b])**.** *Consider the operator*

$$D_{<N} \coloneqq \bigoplus_{3 \leq 2k+1 < N} D_{2k+1} \,.$$

Then the kernel of $D_{<N}$ is $\zeta^{\mathfrak{m}}(N)\mathbb{Q}$ in weight N.

In other words, if the operators D_{2k+1}, for $3 \leq 2k+1 < N$, all simultaneously vanish on a given combination of weight N motivic MZV's. Then this combination is in $\zeta^{\mathfrak{m}}(N)\mathbb{Q}$.

Remark 1.2.16 (Evaluation of the rational)**.** Given some combination X in the kernel of $D_{<N}$, we know from Theorem 1.2.15 that it must be a rational multiple q of $\zeta^{\mathfrak{m}}(N)$.

How can this rational be determined? So far there does not seem to be any conceptual or algorithmic way of determining the rational exactly. Certainly one could determine and combine sufficiently many MZV relations using the regularised double shuffle relations from Section 1.1.4.4. Eventually one should find the exact relation $X - q\zeta(N) = 0$, from which the rational q is now known exactly. However, this is a very impractical way of determining q because the number of relations from regularised double shuffle increases rapidly with the weight, and it becomes difficult to choose the right ones to combine to get the relation $X - q\zeta(N)$.

Instead, the method we will employ to determine this rational q is by numerical evaluation, using the period map. Given some motivic relation, with unknown $q \in \mathbb{Q}$,

$$X - q\zeta^{\mathfrak{m}}(N) = 0 \,,$$

apply the period map to this and rearrange to obtain

$$q = X / \zeta(N) \,.$$

We can then use some algorithms to numerically compute $\zeta(N)$, and the multiple zeta values in X. For example `zetamult`, which is built into recent versions of GP/PARI [GP], can do this. From this, in turn, we can compute q to high accuracy, to hundreds or to thousands of decimal places. We can then find the best rational approximation to this numerical value of q using convergents of the continued fraction of q; this gives the best approximation with the denominator be small compared to the number of decimal places. This approximation can be achieved using the `bestappr` command in GP/PARI [GP].

We can now be pretty sure that we have determined the value of q exactly, although there is of course still the very small chance that we have merely found a very good approximation to it. For more certainty one could recompute the result of $X - q\zeta(N)$ to more and more decimal places, checking the result is 0, to within the error bounds imposed by the `zetamult` algorithm, or compute q to higher accuracy and compare with the initial approximation.

In section 5.3, item iii) of [Bro12b], Brown briefly discusses some potential directions that might eventually lead to an exact way of computing q, such as finding bounds in the prime powers which can appear in the denominator of q, or by finding a different (say, p-adic) realisation of motivic MZV's.

We can give a simple example of these combinatorial tools, as follows. Chapter 2 deals with identities established in the same way for more general and complicated families of MZV's and iterated integrals.

Example 1.2.17. As a simple example of this, we can show that $\zeta^{\mathfrak{m}}(4,4)$ is a rational multiple of $\zeta^{\mathfrak{m}}(8)$.

We have that $\zeta^{\mathfrak{m}}(4,4) = I^{\mathfrak{m}}(0;1,0,0,0,1,0,0,0;1)$. Let us mark out the subsequences for D_3 on $I^{\mathfrak{m}}(0;1,0,0,0,1,0,0,0;1)$ in a table, for clarity. Each term vanishes because the subsequence starts and ends with the same digit – this means the associated integral has equal boundaries so is 0. It is what we called a *trivial* subsequence in Definition 1.2.14.

Subsequence	Term in D_3
$I^{\mathfrak{m}}(\underline{0;1,0,0,0},1,0,0,0;1)$	$I^{\mathfrak{L}}(0;1,0,0;0) \otimes I^{\mathfrak{m}}(0;0,1,0,0,0;1) = 0$
$I^{\mathfrak{m}}(0;\underline{1,0,0,0,1},0,0,0;1)$	$I^{\mathfrak{L}}(1,0,0,0;1) \otimes I^{\mathfrak{m}}(0;1,1,0,0,0;1) = 0$
$I^{\mathfrak{m}}(0;1,\underline{0,0,0,1,0},0,0;1)$	$I^{\mathfrak{L}}(0,0,0,1,0) \otimes I^{\mathfrak{m}}(0;1,0,0,0,0;1) = 0$
$I^{\mathfrak{m}}(0;1,0,\underline{0,0,1,0,0},0;1)$	$I^{\mathfrak{L}}(0,0,1,0,0) \otimes I^{\mathfrak{m}}(0;1,0,0,0,0;1) = 0$
$I^{\mathfrak{m}}(0;1,0,0,\underline{0,1,0,0,0};1)$	$I^{\mathfrak{L}}(0,1,0,0,0) \otimes I^{\mathfrak{m}}(0;1,0,0,0,0;1) = 0$
$I^{\mathfrak{m}}(0;1,0,0,0,\underline{1,0,0,0;1})$	$I^{\mathfrak{L}}(1,0,0,0;1) \otimes I^{\mathfrak{m}}(0;1,0,0,0,1;1) = 0$

Overall we obtain that

$$D_3\zeta^{\mathfrak{m}}(4,4) = 0\,.$$

Let us mark out the subsequences for D_5 on $I^{\mathfrak{m}}(0;1,0,0,0,1,0,0,0;1)$. Two terms in this already vanish because they involve trivial subsequences.

Subsequence	Term in D_5
$I^{\mathfrak{m}}(\underline{0;1,0,0,0,1,0},0,0;1)$	$I^{\mathfrak{L}}(0;1,0,0,0,1,0) \otimes I^{\mathfrak{m}}(0;0,0,0;1) = 0$
$I^{\mathfrak{m}}(0;\underline{1,0,0,0,1,0,0},0;1)$	$I^{\mathfrak{L}}(1,0,0,0,1,0,0) \otimes I^{\mathfrak{m}}(0;1,0,0;1)$
$I^{\mathfrak{m}}(0;1,\underline{0,0,0,1,0,0,0};1)$	$I^{\mathfrak{L}}(0,0,0,1,0,0,0) \otimes I^{\mathfrak{m}}(0;1,0,0;1) = 0$
$I^{\mathfrak{m}}(0;1,0,\underline{0,0,1,0,0,0;1})$	$I^{\mathfrak{L}}(0,0,1,0,0,0;1) \otimes I^{\mathfrak{m}}(0;1,0,0;1)$

So we obtain that

$$D_5\zeta^{\mathfrak{m}}(4,4) = I^{\mathfrak{L}}(1;0,0,0,1,0;0) \otimes I^{\mathfrak{m}}(0;1,0,0;1) + \\ + I^{\mathfrak{L}}(0,0,1,0,0,0;1) \otimes I^{\mathfrak{m}}(0;1,0,0;1)\,.$$

Now apply the reversal of paths property from Property 1.1.13 to the subsequence in the first term of D_5. We have that

$$I^{\mathfrak{L}}(1;0,0,0,1,0;0) = (-1)^5 I^{\mathfrak{L}}(0;0,1,0,0,0;1)\,,$$

so the terms in D_5 cancel, giving

$$D_5\zeta^{\mathfrak{m}}(4,4) = 0\,.$$

Finally, let us mark out the subsequences for D_7 on $I^{\mathfrak{m}}(0;1,0,0,0,1,0,0,0;1)$. Each term in this also vanishes because it involves a trivial subsequence.

Subsequence	Term in D_7
$I^{\mathfrak{m}}(\underbrace{0;1,0,0,0,1,0,0,0};1)$	$I^{\mathfrak{L}}(0;1,0,0;0,1,0,0;0) \otimes I^{\mathfrak{m}}(0;0;1) = 0$
$I^{\mathfrak{m}}(0;\underbrace{1,0,0,0,1,0,0,0;1})$	$I^{\mathfrak{L}}(1;0,0,0,1,0,0,0;1) \otimes I^{\mathfrak{m}}(0;1;1) = 0$

So we obtain that

$$D_7\zeta^{\mathfrak{m}}(4,4) = 0\,.$$

We have computed that $D_{<8}\zeta^{\mathfrak{m}}(4,4) = 0$, so by Theorem 1.2.15, we conclude that $\zeta^{\mathfrak{m}}(4,4) \in \zeta^{\mathfrak{m}}(8)\mathbb{Q}$.

This is confirmed by Identity 1.1.30, where Borwein, Bradley and Broadhurst's result [BBB97] that $\zeta(\{2k\}^n) \in \pi^{2kn}\mathbb{Q}$ is discussed. For this we may write

$$\zeta^{\mathfrak{m}}(4,4) \overset{\mathbb{Q}}{=} \zeta^{\mathfrak{m}}(8)\,,$$

to mean they are equal up to a rational (see Appendix A).

So we have that

$$\zeta^{\mathfrak{m}}(4,4) = q\zeta^{\mathfrak{m}}(8)\,,$$

for some rational $q \in \mathbb{Q}$. By numerically evaluating as in Remark 1.2.16, we can find that $q \approx \frac{1}{12}$ to any accuracy we care to try. So we have that

$$\zeta^{\mathfrak{m}}(4,4) = \frac{1}{12}\zeta^{\mathfrak{m}}(8)\,.$$

Applying the period map to this, we get the corresponding identity on the level of real numbers

$$\zeta(4,4) = \frac{1}{12}\zeta(8) = \frac{32\pi^8}{10!}\,.$$

Remark 1.2.18. The example above is rather trivial in the sense that the exactly identity can be deduced very quickly from the stuffle multiplication. We have

$$\zeta(4)^2 \overset{\text{stuffle}}{=} 2\zeta(4,4) + \zeta(8)\,.$$

Then using Euler's evaluation of $\zeta(2k)$ from Theorem 1.1.6, we get

$$\zeta(4,4) = \frac{1}{2}(\zeta(4)^2 - \zeta(8)) = \frac{1}{2}\left(\left(\frac{\pi^4}{90}\right)^2 - \frac{\pi^8}{9450}\right) = \frac{32\pi^8}{10!}\,.$$

However, the idea of the motivic proof can be generalised to show that $\zeta^{\mathfrak{m}}(\{2k\}^n) \in \zeta^{\mathfrak{m}}(2kn)\mathbb{Q}$, corroborating the evaluations Borwein, Bradley, and Broadhurst produce [BBB97], as discussed in Identity 1.1.30.

A perhaps less trivial identity (in that sense that to obtain it, one needs to more carefully combine various shuffle and stuffle identities) that can be proven motivically (up to $\mathbb{Q}$) is the following.

Example 1.2.19. Consider the combination

$$X = \zeta^{\mathfrak{m}}(1,2,3) + 3\zeta^{\mathfrak{m}}(4,2)\,.$$

I claim that

$$X = \zeta^{\mathfrak{m}}(1,2,3) + 3\zeta^{\mathfrak{m}}(4,2) = \frac{97}{48}\zeta^{\mathfrak{m}}(6)\,.$$

We will show that this is in $\ker D_{<N}$, and then numerically evaluate to find the coefficient $\frac{97}{48}$.

Firstly convert this combination of motivic MZV's to motivic iterated integrals. We get

$$X = -I^{\mathfrak{m}}(0,1,1,0,1,0,0,1) + 3I^{\mathfrak{m}}(0,1,0,0,0,1,0,1)\,.$$

We dispose quickly with the computation of D_5. All of the terms vanish because they already involve a trivial subsequence.

Subsequence	Term in D_5
$-I^{\mathfrak{m}}(\underbrace{0;1,1,0,1,0,0};1)$	$-I^{\mathfrak{L}}(0;1,1,0,1,0;0) \otimes I^{\mathfrak{m}}(0;0;1) = 0$
$-I^{\mathfrak{m}}(0;\underbrace{1,1,0,1,0,0;1})$	$-I^{\mathfrak{L}}(1;1,0,1,0,0;1) \otimes I^{\mathfrak{m}}(0;1;1) = 0$
$3I^{\mathfrak{m}}(\underbrace{0;1,0,0,0,1,0};1)$	$3I^{\mathfrak{L}}(0;1,0,0,0,1;0) \otimes I^{\mathfrak{m}}(0;0;1) = 0$
$3I^{\mathfrak{m}}(0;\underbrace{1,0,0,0,1,0;1})$	$3I^{\mathfrak{L}}(1;0,0,0,1,0;1) \otimes I^{\mathfrak{m}}(0;1;1) = 0$

Now we compute D_3. We will need to make use of the regularisation (as in Section 1.2.3.1) that

$$\begin{aligned} I^{\mathfrak{m}}(0,\underbrace{0}_{k=1},\overbrace{1,0}^{n_1=2},1) &= (-1)^k \sum_{i_1=1} \binom{n_1-1+i_1}{n_i} I^{\mathfrak{m}}(0,1,\{0\}^{n_1-1+i_1},1) \\ &= -2I^{\mathfrak{m}}(0,1,0,0,1) \\ &= 2\zeta^{\mathfrak{m}}(3)\,. \end{aligned}$$

We also need to use $\zeta^{\mathfrak{m}}(1,2) = \zeta^{\mathfrak{m}}(3)$, various instances of reversal of paths, and functoriality under $t \mapsto 1-t$. We obtain the following non-trivial subsequences.

Subsequence	Term in D_3
$-I^{\mathfrak{m}}(0;1,1,0,1,0,0;1)$	$-I^{\mathfrak{L}}(0;1,1,0;1) \otimes I^{\mathfrak{m}}(0;1,0,0;1) = \zeta^{\mathfrak{L}}(3) \otimes \zeta^{\mathfrak{m}}(3)$
$-I^{\mathfrak{m}}(0;1,1,0,1,0,0;1)$	$-I^{\mathfrak{L}}(1;1,0,1;0) \otimes I^{\mathfrak{m}}(0;1,0,0;1) = 2\zeta^{\mathfrak{m}}(3) \otimes \zeta^{\mathfrak{m}}(3)$
$-I^{\mathfrak{m}}(0;1,1,0,1,0,0;1)$	$-I^{\mathfrak{L}}(1;0,1,0;0) \otimes I^{\mathfrak{m}}(0;1,1,0;1) = 2\zeta^{\mathfrak{m}}(3) \otimes \zeta^{\mathfrak{m}}(3)$
$-I^{\mathfrak{m}}(0;1,1,0,1,0,0;1)$	$-I^{\mathfrak{L}}(0;1,0,0;1) \otimes I^{\mathfrak{m}}(0;1,1,0;1) = \zeta^{\mathfrak{m}}(3) \otimes \zeta^{\mathfrak{m}}(3)$
$3I^{\mathfrak{m}}(0;1,0,0,0,1,0;1)$	$3I^{\mathfrak{m}}(0;0,1,0;1) \otimes I^{\mathfrak{m}}(0;1,0,0;1) = -6\zeta^{\mathfrak{m}}(3) \otimes \zeta^{\mathfrak{m}}(3)$

The total contribution to D_3 is therefore 0.

Since both D_3 and D_5 vanish on X, we have that $X \in \ker D_{<N}$, so we obtain

$$X = \zeta^{\mathfrak{m}}(1,2,3) + 3\zeta^{\mathfrak{m}}(4,2) \in \zeta^{\mathfrak{m}}(6)\mathbb{Q}\,,$$

using Theorem 1.2.15. Therefore, there is some $q \in \mathbb{Q}$ such that

$$\zeta^{\mathfrak{m}}(1,2,3) + 3\zeta^{\mathfrak{m}}(4,2) = q\zeta^{\mathfrak{m}}(6)\,.$$

Applying the period map and numerically evaluating as in Remark 1.2.16 shows that $q \approx \frac{97}{48}$, so we get the identity

$$\zeta^{\mathfrak{m}}(1,2,3) + 3\zeta^{\mathfrak{m}}(4,2) = \frac{97}{48}\zeta^{\mathfrak{m}}(6)\,.$$

Applying the period map gives the corresponding identity on the level of real numbers

$$\zeta(1,2,3) + 3\zeta(4,2) = \frac{97}{48}\zeta(6) = \frac{97}{9}\frac{\pi^6}{7!}\,.$$

Further examples of this motivic approach to proving (infinite families of) identities are given in Chapter 2. In Section 2.1.1 we start by revisiting the Broadhurst-Zagier identity and giving a motivic proof that $\zeta(\{1,3\}^n) \in \pi^{4n}\mathbb{Q}$. We then set the Broadhurst-Zagier identity into a broader context, and generalise it to a much larger family of identities which we can prove motivically.

1.2.4 Applications of Brown's motivic MZV's

With this motivic MZV framework, Brown was able to provide a new proof for the bound $\dim_{\mathbb{Q}} \mathcal{Z}_k \leq d_k$ on the dimension of the space of weight k MZV's. However, a more significant application was to provide a proof that the Hoffman elements $\zeta(w)$, with w a word containing only 2's and 3's, span the space of MZV's. This was accomplished by proving that the motivic Hoffman elements are a *basis* for the space of motivic MZV's. This gives some progress towards Conjecture 1.1.37.

We will sketch some of the ideas involved in these proofs. Complete details are found in [Bro12a; Bro12b].

1.2.4.1 Dimension of the space of MZV's

The following is the combination of Lemma 3.3 and Remark 3.7 in [Bro12b]. By the period map, and by construction of $\mathcal{H} \hookrightarrow \mathcal{H}^{\mathcal{MT}+}$, we have:

$$\dim_{\mathbb{Q}} \mathcal{Z}_k \leq \dim_{\mathbb{Q}} \mathcal{H}_k \leq \dim_{\mathbb{Q}} \mathcal{H}_k^{\mathcal{MT}+} .$$

By computing the Poincaré series (the generating series of the dimensions of the graded pieces), we will determine $\dim_{\mathbb{Q}} \mathcal{H}_k^{\mathcal{MT}+} = d_k$. Brown says that $\mathcal{A}^{\mathcal{MT}}$ is non-canonically isomorphic to the cofree Hopf algebra on cogenerators f_{2r+1} in degree $2r+1 \geq 3$, so that the comodule has the following structure:

$$\mathcal{H}^{\mathcal{MT}+} \cong \mathbb{Q}\langle f_3, f_5, \ldots, f_{2r+1}, \ldots \rangle \otimes_{\mathbb{Q}} \mathbb{Q}[f_2]$$

The Poincaré series for $\mathbb{Q}\langle f_3, f_5, \ldots \rangle$ is given by:

$$\frac{1}{1 - t^3 - t^5 - \cdots - t^{2r+1} - \cdots} = \frac{1-t^2}{1-t^2-t^3} .$$

Multiplying this by the Poincaré series for $\mathbb{Q}[f_2]$, which is $\frac{1}{1-t^2}$, gives the Poincaré series for $\mathcal{H}^{\mathcal{MT}+}$ as:

$$\sum_{k \geq 1} \dim_{\mathbb{Q}} \left(\mathcal{H}_k^{\mathcal{MT}+} \right) t^k = \frac{1}{1-t^2} \frac{1-t^2}{1-t^2-t^3} = \frac{1}{1-t^2-t^3} = \sum_{k \geq 1} d_k t^k .$$

So we obtain $\dim_{\mathbb{Q}} \mathcal{H}_k^{\mathcal{MT}+} = d_k$ as required.

This shows that upper bound $\dim_{\mathbb{Q}} \mathcal{Z}_k \leq d_k$ of Zagier's Dimension conjecture, Conjecture 1.1.36 above, does indeed hold.

1.2.4.2 Basis for the space of motivic MZV's, and a spanning set for MZV's

In considering the elements $\zeta^{\mathfrak{m}}$(2's and 3's), Brown is able to show they are linearly independent over $\mathbb{Q}$, [Theorem 7.4 in Bro12a]. Their number in weight k is d_k, so gives the lower bound $\dim_{\mathbb{Q}} \mathcal{H}_k \geq d_k$ on the space of motivic iterated integrals of weight k. Overall this establishes an isomorphism $\mathcal{H} \cong \mathcal{H}^{\mathcal{MT}+}$, not just an embedding.

Brown's proof that $\zeta(w)$, w a word in 2's and 3's, are linearly independent over $\mathbb{Q}$ works inductively on the *level*, defined to be the number of 3's in the word w of the argument of $\zeta^{\mathfrak{m}}$. The base case is provided by the fact that all Hoffman MZV's of level 0, i.e. the elements $\zeta^{\mathfrak{m}}(\{2\}^n)$, are linearly independent over $\mathbb{Q}$. This is clear because they have different weights, so lie in components with different grading.

The induction assumption is that all Hoffman MZV's of level $< \ell$ are linearly independent over $\mathbb{Q}$. Brown shows how a relation between Hoffman MZV's of level ℓ must imply a relation between Hoffman MZV's of strictly smaller level, which contradicts the induction assumption. Establishing this relies heavily on an explicit computation of $\zeta(2, \ldots, 2, 3, 2, \ldots, 2)$ by Zagier [Zag12], and the 2-adic properties of coefficients in this expansion.

The linear independence of $\zeta^{\mathfrak{m}}(w)$, w a word in 2's and 3's, and the number d_k of them in each weight k, means they form a basis for the space of motivic MZV's of weight k. So every motivic MZV can be written as a unique $\mathbb{Q}$-linear combination of these motivic Hoffman elements. Applying the period map shows that the elements Hoffman elements $\zeta(w)$, w a word in 2's and 3's, must *span* the space of classical MZV's, confirming one part of Hoffman's proposed Basis conjecture, Conjecture 1.1.37.

1.2.4.3 Structure of the motivic Galois group $\mathcal{G}_{\mathcal{MT}'}$

Finally, with the previous results Brown settles one conjecture about the structure of the *motivic Galois group* $\mathcal{G}_{\mathcal{MT}'}$ of $\mathcal{MT}'(\mathbb{Z})$. Here $\mathcal{MT}'(\mathbb{Z})$ is the full Tannakian subcategory of $\mathcal{MT}(\mathbb{Z})$ generated by the motivic fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, and $\mathcal{MT}(\mathbb{Z})$ is the category of mixed Tate motives unramified over $\mathbb{Z}$. The conjecture is that the map $\mathcal{G}_{\mathcal{MT}} \twoheadrightarrow \mathcal{G}_{\mathcal{MT}'}$ is an isomorphism, where $\mathcal{G}_{\mathcal{MT}}$ is the motivic Galois group of $\mathcal{MT}(\mathbb{Z})$. A further consequence of this is that the periods of $\mathcal{MT}(\mathbb{Z})$, of mixed Tate motives unramified over $\mathbb{Z}$, are $\mathbb{Q}[\frac{1}{2\pi \mathrm{i}}]$-linear combinations of MZV's.

Chapter 2

Block decomposition of iterated integrals, cyclic insertion on MZV's and motivic identities

In this chapter we introduce a new combinatorial structure on iterated integrals, called the block decomposition (Definition 2.2.4). After defining reflection operators (Definition 2.2.15) and the reflective closure (Definition 2.2.22) of a block decomposition, we show that summing all permutations of these blocks forces the resulting combination to cancel to 0 under Brown's motivic MZV derivation operators D_k. Using Brown's characterisation of $\ker D_{<N}$, this leads to a way of generating infinite families of identities by summing all permutations starting from some arbitrary iterated integral block decomposition ("Symmetric insertion" Theorem 2.4.4).

Numerical experimentation on the resulting identities shows that they typically break up into sums over cyclic shifts of the blocks. This leads to a vast conjectural generalisation ("Generalised cyclic insertion" Conjecture 2.5.1) of the previous Borwein-Bradley-Broadhurst-Lisoněk cyclic insertion conjecture on sums obtained by cyclically inserting blocks of 2 into the MZV $\zeta(\{1,3\}^n)$ (Conjecture 2.1.5). We also obtain a unification with Hoffman's conjectural identity $2\zeta(3,3,\{2\}^n) - \zeta(3,\{2\}^n,1,2) = -\zeta(\{2\}^{n+3})$ (Conjecture 2.1.9). The block decomposition framework is powerful enough to prove Hoffman's identity (up to $\mathbb{Q}$) (Theorem 2.6.5), and produce a symmetrised version of the BBBL cyclic insertion conjecture (Theorem 2.6.2, [Cha15]) which provides something of a refinement to the Bowman-Bradley theorem (Theorem 2.1.7).

We provide many further examples (Section 2.6) of the generalised cyclic insertion conjecture, and the resulting symmetrisations. We focus mainly on identities generated from a subclass of MZV's, which we call 123-MZV's (Definition 2.4.8), because these cyclic/symmetric insertion identities are already sums of MZV's and do not need *regularising*. Moreover, we can describe cyclic insertion on 123-MZV's purely by way of a 'cyclic operator' which manipulates the arguments of the MZV

(Proposition 2.5.12). Finally, we numerically investigate some other identities (Section 2.8) which can be described elegantly in terms of the block decomposition, such as alternating sums over the odd position blocks (Conjecture 2.8.2).

2.1 Background to the cyclic insertion conjecture

We will start by recalling the cyclic insertion conjectured as proposed by Borwein, Bradley, Broadhurst, and Lisoněk, and will set this in its historical context. The cyclic insertion conjecture is obtained by successively generalising an identity of Zagier, by inserting blocks of 2. So far the conjecture has resisted proof, but some limited progress has been made via the Bowman-Bradley theorem which is implied by the conjecture.

2.1.1 Broadhurst-Zagier identity

Firstly, recall the Broadhurst-Zagier identity, which as originally written, states

$$\zeta(\{1,3\}^n) = \frac{2\pi^{4n}}{(4n+2)!} \,.$$

This was conjectured by Zagier on the basis of much numerical evidence in [Zag94]. A proof was later provided by Broadhurst in Section 11 of [BBBL01], using hypergeometric functions. Because of its historical interest it is worth giving the ideas of this proof.

Generating series proof (exact). First interpret $\zeta(\{1,3\}^n)$ as a special value $z = 1$ of the 'single variable' multiple polylogarithm

$$\mathrm{Li}_{s_1,\ldots,s_k}(z) \coloneqq \sum_{0<n_1<n_2<\cdots<n_k} \frac{z^{n_k}}{n_1^{s_1} n_2^{s_2} \cdots n_k^{s_k}} \,.$$

In the paper the notation L is used, and this is defined in terms of a function λ used earlier. To be self-contained I use the above. Then one has

$$\frac{\mathrm{d}}{\mathrm{d}z} \mathrm{Li}_{s_1,\ldots,s_k}(z) = \begin{cases} \frac{1}{z} \mathrm{Li}_{s_1,\ldots,s_k - 1}(z) & \text{if } s_k \geq 2 \\ \frac{1}{1-z} \mathrm{Li}_{s_1,\ldots,s_{k-1}}(z) & \text{if } s_k = 1. \end{cases}$$

In Theorem 11.1 of [BBBL01], Broadhurst shows that

$$\sum_{n=1}^{\infty} \mathrm{Li}_{\{1,3\}^n}(z) t^{4n} = {}_2F_1\left(t\tfrac{(1+\mathrm{i})}{2}, -t\tfrac{(1+\mathrm{i})}{2}; 1; z\right) {}_2F_1\left(t\tfrac{(1-\mathrm{i})}{2}, -t\tfrac{(1-\mathrm{i})}{2}; 1; z\right).$$

Here ${}_2F_1\left(a, b; c; z\right)$ is the Gauss hypergeometric function defined by

$${}_2F_1\left(a, b; c; z\right) \coloneqq \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} z^n \,,$$

and $(q)_n \coloneqq q(q+1)\cdots(q+n-1)$ is the rising Pochhammer symbol.

Broadhurst proves this theorem by noting that both sides of the identity are annihilated by the differential operator

$$\left((1-z)\frac{\mathrm{d}}{\mathrm{d}z}\right)^2 \left(z\frac{\mathrm{d}}{\mathrm{d}z}\right)^2 - t^4 \,,$$

and both sides have the same initial conditions. Namely both sides start

$$1 + \frac{t^4}{8}z^2 + \frac{t^4}{18}z^3 + \frac{t^8+44t^4}{1536}z^4 + O(z^5)\,.$$

In Corollary 2, following this theorem, Broadhurst uses Gauss's ${}_2F_1$ summation theorem to say

$${}_2F_1\left(a,-a;1;1\right) = \frac{\sin(\pi a)}{\pi a}\,.$$

By setting $z=1$ above, Broadhurst obtains

$$\begin{aligned}\sum_{n=0}^\infty \zeta(\{1,3\}^n)t^{4n} &= \frac{2\sin(\frac{1+\mathrm{i}}{2}\pi t)\sin(\frac{1-\mathrm{i}}{2}\pi t)}{\pi^2t^2} \\ &= \frac{\cosh \pi t - \cos \pi t}{\pi^2 t^2} \\ &= \sum_{n=0}^\infty \frac{2\pi^{4n}t^{4n}}{(4n+2)!}\,.\end{aligned}$$

Comparing coefficients of t^{4n} gives Zagier's identity. □

Given the role this will play later, it is also worth noting that a non-explicit version of this result follows readily from Brown's motivic MZV framework. Indeed, in [Bro12b], Brown uses this as an illustration of how much information the operators D_{2r+1} yield about MZV's and their motivic versions. Note, however, that in various versions of [Bro12b] the proof Brown gives is not quite correct.

Motivic proof (up to $\mathbb{Q}$). To show Zagier's identity motivically, it suffices to compute the operators D_{2r+1}, for $r\geq 1$, on $\zeta^{\mathfrak{m}}(\{1,3\}^n)$, and show they all simultaneously vanish. The result follows by Theorem 1.2.15, and applying the period map.

Firstly, as an iterated integral, we have

$$\zeta^{\mathfrak{m}}(\{1,3\}^n) = I^{\mathfrak{m}}(0,\{1,1,0,0\}^n,1)\,.$$

So computing $D_{2r+1}\zeta^{\mathfrak{m}}(\{1,3\}^n)$ involves marking out substrings of length $2r+3$ (recall $2r+1$ is the number of *interior* points) on the word $w \coloneqq 0(1100)^n1$.

Brown claims in [Bro12b] that all subsequences on $I^{\mathfrak{m}}(0;\{1,1,0,0\}^n;1)$ start and end with the same letters, unfortunately this is not correct. Observe that the word w is periodic with period 4. So if r is *odd*, then $2r+2$ is a multiple of 4, and any subsequence of length $2r+3$ on w will start and end with the same letters. So trivially $D_{2r+1}\zeta^{\mathfrak{m}}(\{1,3\}^n)=0$, in this case, and Brown's claim holds.

But, if r is *even*, the subsequences start and end with different letters, and Brown's claim does not hold! However, this is not a problem. Write $r=2s$, and label the positions of the word w starting with the first digit as index 0. For convenience rewrite w as $(0011)^n01$. If the subsequence starts at position i, we obtain different contributions according to the value of $i \pmod 4$.

For example, when $i = 4k$, we mark out the following subsequence

$$\underbrace{(0110)\cdots(0110)}_{k \text{ blocks}}\overbrace{(\mathbf{0110})^{\mathbf{s}}\mathbf{011}}^{\text{subsequence}}\,0\,\underbrace{(0110)\cdots(0110)}_{n-k-s-1 \text{ blocks}}01\,,$$

to obtain the term

$$I^{\mathfrak{L}}((0110)^s011) \otimes I^{\mathfrak{m}}((0110)^k0 \mid 10(0110)^{n-k-s-1}01)$$

in $D_{2r+1}\zeta^{\mathfrak{m}}(\{1,3\}^n)$. In this expression, $|$ is just a notational device to denote the location of the cut out sequence. We will also often drop the commas for notational ease.

Similarly, we obtain the following terms according to $i \pmod 4$:

$$\begin{aligned}
&i = 4k && I^{\mathfrak{L}}((0110)^s011) \otimes I^{\mathfrak{m}}((0110)^k0 \mid 10(0110)^{n-k-s-1}01) \\
&i = 4k+1 && I^{\mathfrak{L}}(110(0110)^s) \otimes I^{\mathfrak{m}}((0110)^k01 \mid 0(0110)^{n-k-s-1}01) \\
&i = 4k+2 && I^{\mathfrak{L}}(10(0110)^s0) \otimes I^{\mathfrak{m}}((0110)^k011 \mid 0110(0110)^{n-k-s-2}01) \\
&i = 4k+3 && I^{\mathfrak{L}}(0(0110)^s01) \otimes I^{\mathfrak{m}}((0110)^k0110 \mid 110(0110)^{n-k-s-2}01)
\end{aligned}$$

Observe that the $I^{\mathfrak{m}}$ factors agree in $i = 4k$ and $i = 4k+1$, and the $I^{\mathfrak{L}}$ factors are reverses of each other. Since the $I^{\mathfrak{L}}$ factors have odd length, they differ by a minus sign. This means the $4k$ term cancels with the $4k+1$ term. Similarly the $I^{\mathfrak{m}}$ factors agree in $i = 4k+2$ and $i = 4k+3$, and the $I^{\mathfrak{L}}$ factors are reverses of each other, so differ by a minus sign. This shows that the $4k+2$ term cancels with the $4k+3$ term. Also note that the last term in D_{2r+1} occurs for i such that $i + (2r+3) - 1 = (4n+2) - 1$, in particular for i odd.

Now $D_{2r+1}\zeta^{\mathfrak{m}}(\{1,3\}^n)$ is the sum of these terms from $i = 0$ to $i = 4n - 2r - 1$. Since the first term has even index, and the last term has odd index, each even index term cancels with the odd index term following it. This means $D_{2r+1}\zeta^{\mathfrak{m}}(\{1,3\}^n)$ cancels completely to give 0.

Since $D_{2r+1}\zeta^{\mathfrak{m}}(\{1,3\}^n)$ is always 0, we find that $\zeta^{\mathfrak{m}}(\{1,3\}^n) \in \ker D_{\leq N}$. By Theorem 1.2.15, we conclude $\zeta^{\mathfrak{m}}(\{1,3\}) \in \zeta^{\mathfrak{m}}(4n)\mathbb{Q}$. Upon taking the period map, we obtain

$$\zeta(\{1,3\}^n) \in \zeta(4n)\mathbb{Q} = \pi^{4n}\mathbb{Q}\,.$$

This proves the claim. □

Before continuing, I wish to slightly rewrite Zagier's identity so that it fits better into the general context. I also want to introduce some convenient notation.

Definition 2.1.1 (wt)**.** In any expression involving MZV's, which is homogeneous in the weight, write wt for the weight.

Example 2.1.2. In Zagier's identity, the weight is $4n$. So with this notation, the identity can be rewritten as follows,

$$\begin{aligned}\zeta(\{1,3\}^n) &= \frac{2\pi^{4n}}{(4n+2)!} \\ &= \frac{\pi^{4n}}{(2n+1)(4n+1)!} \\ &= \frac{1}{2n+1}\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.\end{aligned}$$

2.1.2 Borwein-Bradley-Broadhurst-Lisoněk cyclic insertion conjecture

As we will now explain, later work by Borwein, Bradley, Broadhurst, and Lisoněk (BBBL) has provided a vast conjectural generalisation of this identity. In [BBBL98], these authors manage to prove some special cases of the identity. Bowman and Bradley [BB02] have also proven a family of identities which arises as a consequence of this conjecture.

First let us introduce some notation from [BBBL98] to make writing the identities easier.

Definition 2.1.3. Let $n \in \mathbb{Z}_{\geq 0}$. For $0 \leq i \leq 2n$, let $a_i \in \mathbb{Z}_{\geq 0}$, to obtain a list of $2n+1$ non-negative integers. Then define

$$Z(a_0, \ldots, a_{2n+1}) \coloneqq \zeta(\{2\}^{a_0}, 1, \{2\}^{a_1}, 3, \ldots, 1, \{2\}^{a_{2n-1}}, 3, \{2\}^{a_{2n}})\,.$$

That is, $Z(a_0, \ldots, a_{2n+1})$ is the MZV obtained by inserting the string $\{2\}^{a_i}$ into the i-th gap of the arguments of $\zeta(\{1,3\}^n)$.

Definition 2.1.4. Let n and a_i be as above. Let $\sigma \in S_{2n+1}$, viewed as a permutation of the letters $\{\,0, 1, \ldots, 2n\,\}$. Then we define a version of Z with arguments permuted by σ as follows

$$Z_\sigma(a_0, \ldots, a_{2n}) \coloneqq Z(a_{\sigma(0)}, \ldots, a_{\sigma(2n)})\,.$$

Then BBBL make the following conjecture, which we have slightly rewritten to fit with the notation introduced above.

Conjecture 2.1.5 (BBBL cyclic insertion, Conjecture 1 in [BBBL98])**.** *Let n and a_i be as above. Let $C_{2n+1} = \langle (0\,1\,\cdots\,2n) \rangle$ be the cyclic group of order $2n+1$, viewed as a subgroup of S_{2n+1}. Then*

$$\sum_{\sigma \in C_{2n+1}} Z_\sigma(a_0, \ldots, a_{2n}) \overset{?}{=} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.$$

Here $\overset{?}{=}$ denotes an identity which holds numerically in all cases tested, to several hundred decimal places. (See Appendix A).

This conjecture does indeed represent a generalisation of Zagier's identity. Take $a_0 = a_1 = \cdots = a_{2n} = 0$.

Then we have

$$\begin{aligned} Z(a_0, \ldots, a_{2n}) &= \zeta(\{2\}^0, 1, \{2\}^0, 3, \ldots, 1, \{2\}^0, 3, \{2\}^0) \\ &= \zeta(\{1,3\}^n)\,. \end{aligned}$$

But for any $\sigma \in S_{2n+1}$

$$Z_\sigma(0, 0, \ldots, 0) = Z(0, 0, \ldots, 0)\,.$$

So taking the sum over $\sigma \in C_{2n+1}$, we obtain

$$\begin{aligned} \sum_{\sigma \in C_{2n+1}} Z_\sigma(0, 0, \ldots, 0) &= \sum_{\sigma \in C_{2n+1}} \zeta(\{1,3\}^n) \\ &= (2n+1)\zeta(\{1,3\}^n)\,. \end{aligned}$$

On the other hand, the conjecture would say that

$$\sum_{\sigma \in C_{2n+1}} Z_\sigma(0, 0, \ldots, 0) \stackrel{?}{=} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.$$

Putting these two equalities together gives

$$(2n+1)\zeta(\{1,3\}^n) \stackrel{?}{=} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,,$$

from which Zagier's identity is obtained by dividing through by $2n+1$.

In [BBBL98], Borwein, Bradley, Broadhurst, and Lisoněk manage to prove a special case of this conjecture, which gives Zagier's identity "dressed with 2", as follows.

Theorem 2.1.6 (Theorem 2 in [BBBL98])**.** *The following identity holds*

$$\sum_{\sigma \in C_{2n+1}} Z_\sigma(1, 0, \ldots, 0) = \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.$$

That is the case $a_0 = 1$, $a_1 = a_2 = \cdots = a_{2n+1} = 0$ case of the conjecture holds, as does any cyclically equivalent choice.

The above theorem can be viewed not only as inserting all cyclic permutations of the blocks of 2's given by $\{2\}^1, \{2\}^0, \cdots, \{2\}^0$, but also as inserting all possible blocks of 2's whose total length sum to 1. It is in this direction that Borwein, Bradley, Broadhurst, and Lisoněk have succeeded in proving and explicitly evaluating such combinations of MZV's. This reduces to the previous when $m = 1$.

Theorem 2.1.7 (Bowman-Bradley, Corollary 5.1 in [BB02])**.** *Let $n, m \in \mathbb{Z}_{\geq 0}$ be a non-negative integers. Then*

$$\sum_{\substack{a_0 + \cdots + a_{2n} = m \\ a_i \geq 0}} Z(a_0, a_1, \ldots, a_{2n}) = \frac{1}{2n+1} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!} \binom{m+2n}{2n}\,.$$

It should be noted that the statement in the theorem above is obtained after slightly rewriting the result of Corollary 5.1 in [BBBL98].

Simpler and more refined proofs of this result have since been given by Zhao [Zha08] and Muneta [Mun09].

This result is compatible with the cyclic insertion conjecture. Any composition $\sum_{k=0}^{2n} j_k = m$ of m into $2n+1$ parts remains a composition of m into $2n+1$ parts when cyclically shifted. Hence the terms in the Bowman-Bradley sum can be re-grouped into subsums, where each subsum is taken over a set of compositions which differ by a cyclic shift. Conjecturally, each of these subsums is then a rational multiple of π^{wt}; explicitly it should be $\frac{\alpha}{2n+1} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$, where α is the number of distinct compositions obtained by cyclically shifting a representative composition appearing in this subsum. So on average each of the $\binom{m+2n}{2n}$ compositions contributes $\frac{1}{2n+1} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$, giving a total which agrees with the above.

2.1.3 Family of evaluable MZV's

If the BBBL cyclic insertion conjecture is true, then one consequence will be the evaluability of a certain two-parameter family of MZV's, for which Zagier's $\zeta(\{1,3\}^n)$ is one of the simplest examples. This family was conjectured by Borwein, Bradley, and Broadhurst in [BBB97].

Conjecture 2.1.8 (Equation 18 of [BBB97])**.** *Let $n, m \in \mathbb{Z}_{\geq 0}$ be non-negative integers. Then*

$$\zeta(\{\{2\}^m, 1, \{2\}^m, 3\}^n, \{2\}^m) \stackrel{?}{=} \frac{1}{2n+1} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!} \,.$$

This family is obtained as the $a_0 = a_1 = \cdots = a_{2n} = m$ case of the cyclic insertion conjecture. And in the case where $m = 0$, we recover Zagier's identity.

2.1.4 Hoffman's identity

Another conjectural family of identities, attributed to Hoffman in equation 5.6 of [BZ], is the following

Conjecture 2.1.9 (Hoffman)**.** *Let $n \in \mathbb{Z}_{\geq 0}$ be a non-negative integer. Then*

$$2\zeta(3,3,\{2\}^n) - \zeta(3,\{2\}^n,1,2) \stackrel{?}{=} -\zeta(\{2\}^{n+3}) = -\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!} \,.$$

This family of identities has much the same flavour as the cyclic insertion conjecture. A certain length block $\{2\}^n$ is inserted into some MZV's, and the resulting sum is (up to sign) $\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$. This result has been checked up to weight 22, where $n = 8$, using tables of known MZV relations by Vermaseren [BZ].

2.1.5 Unification of identities and progress towards proofs

It turns out that Hoffman's identity, and the BBBL cyclic insertion conjecture, both arise from the same procedure applied to (what I call) the *block decomposition* of an MZV. That is to say, both of these conjectural identities are part of the same, and indeed much larger, family of conjectural identities.

The goal of this chapter is therefore two-fold. Firstly, we want to illustrate the procedure which unifies these two families of identities into a generalised cyclic insertion conjecture (Conjecture 2.5.1). Secondly, although we cannot prove this generalised conjecture exactly, we will use Brown's motivic MZV framework to show that a sufficiently symmetrised version of the identity holds up to a rational (Theorem 2.5.4).

I proved this for the original BBBL cyclic insertion conjecture much earlier, and this was written up and published in [Cha15]. The results here for the general cyclic insertion conjecture are therefore new. The main result in [Cha15], Theorem 2.6.2 below, becomes a simple consequence of Theorem 2.5.4.

In Section 5.10 of [Zha16], Zhao notes that "by a tedious computation" using the idea of [Cha15], Hoffman's identity can indeed be proved up to $\mathbb{Q}$. In what follows, we will establish a general framework by which Hoffman's identity can be proven, and indeed generalised (Conjecture-Example 2.6.6 and its symmetrisation, Theorem 2.6.7), by quick and elegant calculations on *block decompositions*.

2.2 Block decomposition and reflection operators

2.2.1 Block decomposition of iterated integrals

In order to formulate a generalisation of the BBBL cyclic insertion conjecture, and to prove some results in this direction, we need to introduce a new way of encoding/describing MZV's, and by extension iterated integrals over the alphabet $\{ 0, 1 \}$.

Firstly, we introduce notation for the two basic strings which serve as building-blocks for the words over $\{ 0, 1 \}$, which define the iterated integrals.

Definition 2.2.1 (Strings W_0 and W_1)**.** Let W_0 denote the (infinite) string

$$W_0 \coloneqq 01010101\ldots\,,$$

consisting of an alternating sequence of 0's and 1's, beginning with a 0. And let W_1 denote the (infinite) string

$$W_1 \coloneqq 10101010\ldots\,,$$

consisting of an alternating sequence of 1's and 0's, beginning with a 1.

We write W_i^ℓ to denote the string obtained by taking the first ℓ letters of W_i.

Notation 2.2.2. Given two words w and u over the alphabet $\{ 0, 1 \}$, the concatenation of w and u can be denoted simply by the juxtaposition wu. For emphasis it may be denoted using $\oplus$, as in $w \oplus u$.

Lemma 2.2.3. *Let w be a word over $\{ 0, 1 \}$. Then the word w can be expressed as a concatenation of words of the form $W_i^{\ell_i}$, for $i = 1, \ldots, n$, where the last letter of $W_j^{\ell_j}$ agrees with first letter of $W_{j+1}^{\ell_{j+1}}$. Moreover, this representation is unique.*

Proof. It is of course trivial that w can be expressed as a concatenation of W_0's and W_1's because $W_0^1 = 0$ and $W_1^1 = 1$. Requiring that the last digit of $W_j^{\ell_j}$ agrees with the first digit of $W_{j+1}^{\ell_{j+1}}$ is less trivial.

Uniqueness: First let us deal with the uniqueness claim. Suppose that $B_1 = W_{\epsilon_1}^{\ell_1} \oplus \cdots \oplus W_{\epsilon_n}^{\ell_n}$ and $B_2 = W_{\delta_1}^{k_1} \oplus \cdots \oplus W_{\delta_m}^{k_m}$ are two (ostensibly) different decompositions of w, satisfying the above conditions. We want to show that $n = m$, and that $\delta_i = \epsilon_i$ and $k_i = \ell_i$, for $i = 1, \ldots, n$.

We may remove any leading terms $W_j^{\ell_j}$ from B_1 and B_2 which happen to agree. If this leaves two copies of the empty word, we are done, so we assume that it does not.

This procedure cannot result in only one copy of the empty word. Suppose B_1 leaves an empty word $B_1' = \emptyset$, but B_2 leaves a non-empty word B_2'. Then B_1' and B_2' have different lengths, respectively 0 and > 0. We obtain the original words B_1 and B_2 by prepending the same word, $B_0 = W_{\epsilon_1}^{\ell_1} \oplus W_{\epsilon_{n'}}^{\ell_{n'}}$ of length L to both. This will mean B_1 has length $0 + L = L$, and B_2 has length $> 0 + L = L$. This shows that B_1 and B_2 cannot express the same word.

So after removing any identical leading terms, we may assume that the first difference between B_1 and B_2 occurs in the first term. Since the words described by B_1 and B_2 are equal, their first letters in particular are equal. Therefore we have $\epsilon_1 = \delta_1$. Now consider the lengths ℓ_1 and k_1. Since there is a difference in the first term, we must have $\ell_1 \neq k_1$, and by swapping $B_1 \leftrightarrow B_2$, we can assume that $\ell_1 < k_1$.

Now compute the letter at position $\ell_1 + 1$. Using B_1, we find this is equal to the $\epsilon_1 + (\ell_1 - 1) \pmod 2$, as illustrated

$$(\underbrace{0101\ldots01}_{\ell_1 \text{ symbols}})(\underbrace{1}_{\text{position } \ell_1+1}0\ldots10)\,.$$

But using B_2, we find that is is equal to $\delta_1 + (\ell_1) \pmod 2$, as illustrated

$$(\underbrace{0101\ldots01}_{\ell_1 \text{ symbols}}\underbrace{0}_{\text{position } \ell_1+1}\ldots)\,.$$

Since these must be equal, we must have $\epsilon_1 + (\ell_1 - 1) = \delta_1 + (\ell_1) \pmod 2$. Knowing $\epsilon_1 = \delta_1$, this entails $0 = 1 \pmod 2$, a contradiction.

We conclude, then, that it is not possible to have two different decompositions for the word w.

Existence: Now let us show that such a decomposition does indeed exist. This will be by induction. We can explicitly check the case where w has length $L = 1$, since

$$w = 0 \text{ decomposes as } W_0^1, \text{ and}$$

$$w = 1 \text{ decomposes as } W_1^1.$$

Suppose now that all words of length $< L$ can be so decomposed. Let w be a word of length L. If w does not contain the substring 00, and does not contain the substring 11, then w must be an alternating sequence of 0's and 1's. Therefore $w = W_{\epsilon_1}^L$, where ϵ_i is the first digit of w.

Otherwise, we can find the first occurrence of 00 or 11 in w. We split w into w_1 and w_2 at this point, so that w_1 ends at the first 0 of 00, and w_2 starts at the second 0 or 00. (Or the equivalent if we find 11 occurs first.) Since w_2 has length $< L$, we can decompose it as $W_{\epsilon_2}^{\ell_2} \oplus \cdots \oplus W_{\epsilon_n}^{\ell_n}$, using the induction hypothesis. As w_1 does not contain the substring 00 and does not contain the substring 11 (since we cut in the middle of the first such occurrence), we can express it as $w_1 = W_{\epsilon_1}^{\ell_1}$ for some ϵ_1 and some ℓ_1, as above.

Since the first digit of $W_{\epsilon_2}^{\ell_2}$ agrees with the last digit of $W_{\epsilon_1}^{\ell_1}$ by construction, we can put these together to obtain

$$w = W_1^{\ell_1} \oplus \cdots \oplus W_n^{\ell_n} \,,$$

as a decomposition for w. This completes the proof. □

Definition 2.2.4 (Block decomposition)**.** Let w be a word over $\{ 0, 1 \}$, and let

$$w = W_{\epsilon_1}^{\ell_1} \oplus \cdots \oplus W_{\epsilon_n}^{\ell_n}$$

be the decomposition of w as produced by Lemma 2.2.3. We define the *block decomposition* of w to be

$$\operatorname{block}(w) \coloneqq (\epsilon_1;\ \ell_1, \ldots, \ell_n) \,.$$

If $\epsilon_1 = 0$, then we may write $(\ell_1, \ldots, \ell_n)$ instead of $(0; \ell_1, \ldots, \ell_n)$.

Remark 2.2.5. Notice that only ϵ_1 is required in this description. We can calculate ϵ_{i+1} from ϵ_i by knowing that the first digit of $W_{\epsilon_{i+1}}^{\ell_{i+1}}$ is equal to the last digit of $W_{\epsilon_i}^{\ell_i}$. The last digit of $W_{\epsilon_i}^{\ell_i}$ is $\epsilon_i + (\ell_i - 1) \pmod 2$, so $\epsilon_{i+1} = \epsilon_i + (\ell_i - 1) \pmod 2$. We can therefore recover w from $\operatorname{block}(w)$.

Definition 2.2.6 (word)**.** Given a block decomposition $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$, we will write

$$\operatorname{word}(B) \coloneqq W_{\epsilon_1}^{\ell_1} \oplus \cdots \oplus W_{\epsilon_n}^{\ell_n} \,.$$

This recovers the word which gives the indicated block decomposition.

Remark 2.2.7. It will often be helpful to use the block and word functions to identify a block decomposition with the word it encodes. That is, give a word w and a block decomposition B, we may write $B = w$ to mean $\operatorname{word}(B) = w$, or equivalently $B = \operatorname{block}(w)$.

Definition 2.2.8 (Block integral, number of blocks)**.** Given a block decomposition $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$, we define the *block integral* $I_{\mathrm{bl}}^{\mathfrak{m}}(B)$ as follows:

$$I_{\mathrm{bl}}^{\mathfrak{m}}(B) \coloneqq I^{\mathfrak{m}}(\operatorname{word}(B)) \,.$$

We shall call n the *number of blocks* in the integral.

If $\epsilon_1 = 0$, we may write

$$I^{\mathfrak{m}}_{\mathrm{bl}}(\ell_1, \ldots, \ell_n) \coloneqq I^{\mathfrak{m}}_{\mathrm{bl}}(0;\ \ell_1, \ldots, \ell_n) = I^{\mathfrak{m}}(\mathrm{word}(0;\ \ell_1, \ldots, \ell_n))$$

for simplicity.

Example 2.2.9. Suppose, for example, we take the integral

$$I^{\mathfrak{m}}(w) = I^{\mathfrak{m}}(001010011101010110011)\,.$$

We find that the word w can be decomposed as follows

$$\begin{aligned} w &= (0) \oplus (01010) \oplus (01) \oplus (1) \oplus (1010101) \oplus (10) \oplus (01) \oplus (1) \\ &= W_0^1\, W_0^5\, W_0^2\, W_1^1\, W_1^7\, W_1^2\, W_0^2\, W_1^1\,. \end{aligned}$$

Therefore the block decomposition of w is given by

$$\mathrm{block}(w) = (0;\ 1, 5, 2, 1, 7, 2, 2, 1)\,.$$

As a block integral, we have the following. Here the separators $|$ are just a visual device to make identifying the blocks more straightforward.

$$\begin{aligned} I^{\mathfrak{m}}(w) &= I^{\mathfrak{m}}(0 \mid 01010 \mid 01 \mid 1 \mid 1010101 \mid 10 \mid 01 \mid 1) \\ &= I^{\mathfrak{m}}_{\mathrm{bl}}(0;\ 1, 5, 2, 1, 7, 2, 2, 1) \\ &= I^{\mathfrak{m}}_{\mathrm{bl}}(1, 5, 2, 1, 7, 2, 2, 1)\,, \end{aligned}$$

since $\epsilon_1 = 0$. This integral consists of 8 blocks.

Notation 2.2.10. It is convenient to introduce some notation to refer directly to different aspects of the i-th block of a block decomposition. Let $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$ be a block decomposition. We will write $B_i^{\mathrm{L}} \coloneqq \ell_i$ to mean the length of the i-th block. We shall write B_i^{st} to mean the initial digit of the i-th block, that is $B_i^{\mathrm{st}} \coloneqq \epsilon_i$. We shall also write B_i^{en} to mean the final digit of the i-th block, so that $B_i^{\mathrm{en}} \coloneqq \epsilon_i + (\ell_i - 1) \pmod 2$.

Here we collect some simple facts about the block integral, and block decompositions.

Lemma 2.2.11. *Let $I^{\mathfrak{m}}_{\mathrm{bl}}(\epsilon_1;\ \ell_1, \ldots, \ell_n)$ be a block integral. Then the integral has weight $-2 + \sum_i \ell_i$. We use this connection to define the* weight *of a block decomposition as $-2 + \sum_i \ell_i$*

Proof. The word $w = \mathrm{word}(\epsilon_1;\ \ell_1, \ldots, \ell_n)$ has length $\sum_i \ell_i$ because the i-th block has length ℓ_i. But this word includes the upper and lower bound of the iterated integral $I^{\mathfrak{m}}(w)$, which we must discount. So the weight is $-2 + \sum_i \ell_i$. ☐

Lemma 2.2.12. *Let $I = I^{\mathfrak{m}}_{\mathrm{bl}}(B)$ be a block integral with weight t and n blocks. Then the upper and lower bounds are equal, meaning $I^{\mathfrak{m}}_{\mathrm{bl}}(B) = 0$, if and only if $t = n \pmod 2$. Such a block decomposition B will be called* non-trivial *if the upper and lower bounds of the corresponding integral are different.*

Remark 2.2.13. It is interesting to compare the structure of this with Tsumura's depth-partiy theorem [Tsu04]. Both results have that form that an object simplifies (to zero in this case, or to lower depth in Tsumura's case) if some parity condition holds (equal parity in this case, and opposite parity in Tsumura's case). Of course this result is just a trivial observation that the bounds of integration are equal, whereas [Tsu04]'s result is highly non-trivial.

Proof of Lemma 2.2.12. Say $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$. Then first letter of I is ϵ_1, this is the lower bound of $I^{\mathfrak{m}}_{\mathrm{bl}}(B)$.

We claim that the first letter of the j-th block is $\epsilon_1 + \sum_{i=1}^{j-1}(\ell_i - 1) \pmod 2$. This can be shown by induction. In the case $j = 1$, we obtain the first digit as $\epsilon_1 + \sum_{i=1}^{0}(\ell_i - 1) = \epsilon_1$. Suppose this holds for $j-1$. Then we know that $B_j^{\mathrm{st}} = B_{j-1}^{\mathrm{en}}$, and $B_{j-1}^{\mathrm{en}} = B_{j-1}^{\mathrm{st}} + (B_{j-1}^{\mathrm{L}} - 1)$. Therefore we get for j

$$\begin{aligned} B_j^{\mathrm{st}} = B_{j-1}^{\mathrm{st}} + (B_{j-1}^{\mathrm{L}} - 1) &= (\epsilon_1 + \sum_{i=1}^{j-2}(\ell_i - 1)) + (\ell_{j-1} - 1) \\ &= \epsilon_1 + \sum_{i=1}^{j-1}(\ell_i - 1) \pmod 2 \,. \end{aligned}$$

So the last letter of the n-th block is

$$\begin{aligned} B_n^{\mathrm{en}} = B_n^{\mathrm{st}} + (\ell_n - 1) &= \epsilon_1 + \sum_{i=1}^{n-1}(\ell_i - 1) + (\ell_n - 1) \\ &= \epsilon_1 + \sum_{i=1}^{n}(\ell_i - 1) = \epsilon_1 - 2 + t - n \pmod 2 \,. \end{aligned} \tag{2.2.1}$$

So the last letter of I is $\epsilon_1 + t - n \pmod 2$, this is the upper bound of $I^{\mathfrak{m}}_{\mathrm{bl}}(B)$. This is equal to the lower bound ϵ_1 if and only if $t - n = 0 \pmod 2$, which is if and only if $t = n \pmod 2$. ☐

Lemma 2.2.14. *Let $I = I^{\mathfrak{m}}_{\mathrm{bl}}(B)$ be a block integral with n blocks and weight t. Suppose that $t \neq n \pmod 2$, and $t \geq 2$. Then I is divergent if and only if $B_1^{\mathrm{L}} = 1$ or $B_n^{\mathrm{L}} = 1$.*

Proof. Recall from Section 1.1.3 that an integral $I^{\mathfrak{m}}(a_0; a_1, \ldots, a_m; a_{m+1})$ with weight $m \geq 2$ amd $a_0 \neq a_{m+1}$ is said to be *divergent* if $a_0 = a_1$ or $a_m = a_{m+1}$. The condition $t \neq n \pmod 2$ is equivalent to $a_0 \neq a_{m+1}$, and $t \geq 2$ is equivalent to $m \geq 2$.

If $B_1^{\mathrm{L}} = 1$, $B_2^{\mathrm{st}} = B_1^{\mathrm{en}} = B_1^{\mathrm{st}}$, so $\mathrm{word}(B) = W_{\epsilon_1}^1 W_{\epsilon_1}^{\ell_2} \oplus \cdots$, which starts $\epsilon_1\epsilon_1\cdots$. So $a_0 = a_1$, and the integral is divergent. Similarly if $B_n^{\mathrm{L}} = 1$, then $B_{n-1}^{\mathrm{en}} = B_n^{\mathrm{st}} = B_n^{\mathrm{en}}$. So $\mathrm{word}(B) = \cdots \oplus W_{\epsilon_{n-1}} W_{\epsilon_n}^1$, which ends $\cdots\epsilon_n\epsilon_n$. This means $a_m = a_{m-1}$ and the integral is divergent.

On the other hand, if $B_1^{\mathrm{L}} > 1$ and $B_n^{\mathrm{L}} > 1$, then $\mathrm{word}(B) = W_{\epsilon_1}^{>1} \oplus \cdots \oplus W_{\epsilon_n}^{>1}$ which starts $(\epsilon_1)(1-\epsilon_1)\cdots$ and ends $\cdots(1-\epsilon_1)(\epsilon_1)$. This means $a_0 \neq a_1$ and $a_m \neq a_{m+1}$, and the integral is not divergent. ☐

2.2.2 Reflection operators

We are now going to define reflection operators on the set of all words over $\{0,1\}$, via their block encoding. Later, this will be lifted to define a reflection operator on subsequences of words, in order to compute the derivations D_{2r+1} as applied to some combination of motivic iterated integrals.

Definition 2.2.15 (Reflection $\mathcal{R}_{j,k}$)**.** Let $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$ be a block decomposition with n blocks. For each $1 \leq j < k \leq n$, we define the reflection operator $\mathcal{R}_{j,k}$ as follows. We set $\mathcal{R}_{j,k} B \coloneqq (\epsilon'_1;\ \ell'_1, \ldots, \ell'_n)$, where $\epsilon'_1 \coloneqq \epsilon_1$, and

$$\ell'_i \coloneqq \begin{cases} \ell_i & \text{for } i < j, \text{ or } i > k, \text{ and} \\ \ell_{k+j-i} & \text{for } j \leq i \leq k. \end{cases}.$$

We then set $\mathcal{R}_{j,k} w \coloneqq \operatorname{word}(\mathcal{R}_{j,k} \operatorname{block}(w))$ to define the reflection operators directly on words over $\{0,1\}$.

This operator reverses the block lengths from positions j to k, inclusive.

Remark 2.2.16. The duality relation on MZV's and iterated integrals is closely related with the reflection operator $\mathcal{R}_{1,n}$, which reflects an entire block decomposition B consisting of n blocks.

Assuming that $B = (\epsilon_1; \ell_1, \ldots, \ell_n)$ is a non-trivial block decomposition (in the sense of Lemma 2.2.12) with n blocks and weight t. Then the dual to the integral $I^{\mathfrak{m}}_{\mathrm{bl}}(B) = I^{\mathfrak{m}}_{\mathrm{bl}}(\epsilon_1; \ell_1, \ldots, \ell_n)$ is the integral $(-1)^t I^{\mathfrak{m}}_{\mathrm{bl}}(\mathcal{R}_{1,n} B) = (-1)^t I_{\mathrm{bl}}(\epsilon_1; \ell_n, \ldots, \ell_1)$.

Lemma 2.2.17. *The reflection operator $\mathcal{R}_{j,k}$ preserves the weight, and number of blocks, when applied to a block decomposition B.*

Proof. This is clear by the definition of $\mathcal{R}_{j,k}$ on the block decomposition $B = \operatorname{block}(w) = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$. The result of $\mathcal{R}_{jk} B$ is another block decomposition with n blocks, and the weight is still $-2 + \sum_i \ell_i$, although the ℓ_i are summed in a different order. ☐

Lemma 2.2.18. *Where defined, the operator $\mathcal{R}_{j,k}$ is an involution. So for $1 \leq j < k \leq n$, each $\mathcal{R}_{j,k}$ defines an automorphism on the set*

$$\{ B \mid B \textit{ has } n \textit{ blocks} \}$$

of block decompositions with n blocks.

Proof. Let $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$, and $1 \leq j < k \leq n$ be given. Say that $\mathcal{R}_{jk} B = (\epsilon'_1;\ \ell'_1, \ldots, \ell'_n)$. Then $\mathcal{R}_{j,k}$ is defined on $\mathcal{R}_{j,k} B$. So suppose $\mathcal{R}_{jk} \mathcal{R}_{jk} B = (\epsilon''_1;\ \ell''_1, \ldots, \ell''_n)$.

By definition we know that $\epsilon''_1 = \epsilon'_1 = \epsilon_1$. Now look at ℓ''_i. For $i < j$, or $i > k$, we have that $\ell''_i = \ell'_i = \ell_i$. For $j \leq i \leq k$ we have $\ell''_i = \ell'_{k+j-i}$. But notice that $j \leq k + j - i \leq k$, for this range of i. We therefore compute $\ell'_{k+j-i} = \ell_{k+j-(k+j-i)} = \ell_i$.

Overall this means $\ell''_i = \ell_i$, for all $1 \leq i \leq n$. Hence $\mathcal{R}_{jk} \mathcal{R}_{jk} B = B$, and the claim is proved. ☐

Example 2.2.19. Consider again the integral from Example 2.2.9,

$$I^{\mathfrak{m}}(w) = I^{\mathfrak{m}}(0 \mid 01010 \mid 01 \mid 1 \mid 1010101 \mid 10 \mid 01 \mid 1)\,.$$

The word w describing this integral has block decomposition

$$B = \operatorname{block}(w) = (0;\ 1, 5, 2, 1, 7, 2, 2, 1)\,.$$

We can compute $\mathcal{R}_{2,5}B$ to be

$$\mathcal{R}_{2,5}B = (0;\ 1, \underbrace{7, 1, 2, 5}_{\text{reversed}}, 2, 2, 1)\,.$$

This is the block encoding of the word

$$\operatorname{word}(\mathcal{R}_{2,5}B) = (0)(0101010)(0)(01)(10101)(10)(01)(1)\,.$$

Later one, in Section 2.2.4 and Section 2.3 we will use the $\mathcal{R}_{j,k}$ to define a reflection operator $\mathcal{R}$ on subsequences of words, and use this to cancel terms in $D_{<N}$. Thus we will be able to cancel a subset of terms in $D_{<N}$ between

$$\begin{gathered} I^{\mathfrak{m}}(0 \mid 01010 \mid 01 \mid 1 \mid 1010101 \mid 10 \mid 01 \mid 1) \text{ and} \\ I^{\mathfrak{m}}(0 \mid \underbrace{0101010 \mid 0 \mid 01 \mid 10101}_{\text{reversed}} \mid 10 \mid 01 \mid 1) \\ = I^{\mathfrak{m}}(\mathcal{R}_{2,5}\, 0 \mid 01010 \mid 01 \mid 1 \mid 1010101 \mid 10 \mid 01 \mid 1)\,. \end{gathered}$$

Remark 2.2.20. The reflection operator $\mathcal{R}_{j,k}$ is only defined on words, and not in the motivic iterated integrals themselves. This is because these the reflection operators and block decompositions do not respect the relations satisfied by motivic iterated integrals.

Indeed, even the number of blocks is not preserved under all relations, as the follow shows. The MZV $\zeta(\{1,3\}^n)$ has block decomposition

$$\zeta^{\mathfrak{m}}(\{1,3\}^n) = I^{\mathfrak{m}}(01 \mid 10 \mid \cdots \mid 01) = I^{\mathfrak{m}}_{\mathrm{bl}}(\{2\}^{2n+1})\,,$$

consisting of $2n+1$ blocks of length 2. Whereas the MZV $\zeta(\{2\}^{2n})$ has block decomposition

$$\zeta^{\mathfrak{m}}(\{2\}^{2n}) = I^{\mathfrak{m}}(0101\ldots01) = I^{\mathfrak{m}}_{\mathrm{bl}}(4n+2)\,,$$

consisting of a single block of length $4n+2$. However, by the Broadhurst-Zagier identity (Identity 1.1.31), we get the following equality

$$(2n+1)I^{\mathfrak{m}}_{\mathrm{bl}}(\{2\}^{2n+1}) = I^{\mathfrak{m}}_{\mathrm{bl}}(4n+2)\,,$$

which relates a 1 block integral, and a $2n+1$ block integral.

In the above case, the reflection operator $\mathcal{R}_{1,2n+1}$ is defined for the block decomposition $B_1 = (0; \{2\}^{2n+1})$. However, $\mathcal{R}_{1,2n+1}$ it is not defined on the block decomposition $B_2 = (0; 4n+2)$, even though the corresponding integrals are equal (up to a rational multiple).

By abuse of notation, we *could* extend the notion of reflection operators to integral $I^{\mathfrak{m}}(w)$. However, this would only be with the understanding that the reflection operator act on the particular choice of word w appearing as the argument of the iterated integral. We would not be allowed to use *any* relations rewrite $I^{\mathfrak{m}}(w)$ in another form, before computing $\mathcal{R}_{j,k}$.

2.2.3 Reflectively closed sets

We are now in a position to define the main objects which will be used to create identities on iterated integrals and MZV's.

Definition 2.2.21 (Reflectively closed sets)**.** Let S be a subset of

$$\{ B \mid B \text{ is a block decomposition, with } n \text{ blocks, and weight } t \} .$$

We say that S is *reflectively closed* if for every $B \in S$, the result of $\mathcal{R}_{j,k}B$ is already in S, for $i \leq j < k \leq n$.

Definition 2.2.22 (Reflective closure)**.** Let S be a subset of

$$\{ B \mid B \text{ is a block decomposition, with } n \text{ blocks, and weight } t \} .$$

We define the *reflective closure* of S, written $\langle S \rangle_{\mathcal{R}}$, to be the smallest reflectively closed set containing S. That is, $\langle S \rangle_{\mathcal{R}}$ is such that $\langle S \rangle_{\mathcal{R}}$ is a subset of any other reflectively closed set containing S.

Remark 2.2.23. Using the identification in Remark 2.2.7, we may extend the notion of reflective closure from block decompositions B to words w whose block decompositions have a fixed number of blocks n, and fixed weigh t.

Proposition 2.2.24. *Let S be a subset of*

$$H \coloneqq \{ B \mid B \textit{ is a block decomposition, with } n \textit{ blocks, and weight } t \} .$$

Then the reflective closure of S exists, and it may be computed as the intersection of all reflectively closed sets containing S.

Proof. Observe that some reflectively closed set containing S does indeed exist. We may take that set to be all of H. Since $\mathcal{R}_{j,k}$ preserves the weight, and number of blocks, in an iterated integral, we certainly have $\mathcal{R}_{j,k}B \in H$, for every $B \in H$, and every $1 \leq j < k \leq n$.

We show that the intersection of a family of reflectively closed sets containing S is a reflectively closed set containing S. Let $\mathcal{F}$ be such a family. Then we have $S \subset F$ for every $F \in \mathcal{F}$, so that $S \subset \bigcap \mathcal{F}$. Moreover, let $B \in \bigcap \mathcal{F}$, then $B \in F$ for every $F \in \mathcal{F}$. But by the reflective closure of F we see that $\mathcal{R}_{j,k}B \in F$, so $\mathcal{R}_{j,k}B \in F$ for every $F \in \mathcal{F}$, and we conclude $\mathcal{R}_{j,k}B \in \bigcap \mathcal{F}$. Therefore $\mathcal{F}$ is a reflectively closed set containing S.

Finally let $\mathcal{F} = \{\, F \mid F \text{ is a reflectively closed set containing } S \,\}$. We show that

$$T = \bigcap \mathcal{F}$$

is the reflective closure of S. Certainly we know that T is a reflectively closed set containing S. We show that it is the smallest. Let U be another reflectively closed set containing S. Then $U \in \mathcal{F}$, so that $\bigcap \mathcal{F} \subset U$. Therefore $T \subset U$. Thus we have $T = \langle S \rangle_{\mathcal{R}}$. □

Example 2.2.25. Consider the word $w = 0101001101$ which describes the iterated integral $I^{\mathfrak{m}}(0101001101) = \zeta^{\mathfrak{m}}(2,3,1,2)$. The word w has block decomposition $B = (0;5,2,3) = (5,2,3)$. The block decomposition B has weight 8, and consists of 3 blocks. If we continually apply $\mathcal{R}_{j,k}$ to this block decomposition, and all subsequently generated block decompositions, we find the following set of block decompositions.

$$\begin{aligned} \widetilde{S} = \{\, & (0;3,5,2), (0;3,2,5), (0;5,3,2), \\ & (0;5,2,3), (0;2,5,3), (0;2,3,5) \,\} \end{aligned}$$

Upon using the identification between block decompositions and words from Remark 2.2.7, we can say this is

$$\begin{aligned} = \{\, & 010 \mid 01010 \mid 01, \quad 010 \mid 01 \mid 10101, \quad 01010 \mid 010 \mid 0, \\ & 0101 \mid 001 \mid 101, \quad 01 \mid 10101 \mid 101, \quad 01 \mid 101 \mid 10101 \,\} \,. \end{aligned}$$

One can check that this set S is indeed reflectively closed. Moreover, since every element of this arises by applying some sequence of reflection operators $\mathcal{R}_{j,k}$, this is the smallest possible reflectively closed set containing 0101001101. Therefore

$$\widetilde{S} = \langle (0;5,2,3) \rangle_{\mathcal{R}} = \langle 01010 \mid 01 \mid 101 \rangle_{\mathcal{R}} \,.$$

As a foreshadowing of what is to come in Theorem 2.3.8 and Corollary 2.3.9, let us integrate these block decompositions, and convert the results back to MZV's. Remembering the $(-1)^{\text{depth}}$, we obtain the following set of MZV's

$$\begin{aligned} S = \{ & -\zeta^{\mathfrak{m}}(3,2,3), \zeta^{\mathfrak{m}}(3,1,2,2), -\zeta^{\mathfrak{m}}(2,3,3), \\ & \zeta^{\mathfrak{m}}(2,3,1,2), -\zeta^{\mathfrak{m}}(1,2,2,1,2), -\zeta^{\mathfrak{m}}(1,2,1,2,2) \} \,. \end{aligned}$$

It turns out that

$$\sum\nolimits_{s \in \widetilde{S}} I^{\mathfrak{m}}_{\text{bl}}(s) = \sum\nolimits_{s \in S} s = 2\zeta^{\mathfrak{m}}(2,2,2,2) \in \zeta^{\mathfrak{m}}(8)\mathbb{Q} \,,$$

so in particular

$$\text{per}\left(\sum\nolimits_{s \in S} s \right) = 2\zeta(2,2,2,2) = 2\frac{\pi^8}{9!} \in \zeta(8)\mathbb{Q} = \pi^8\mathbb{Q} \,.$$

Here the weight is low enough that a brute force evaluation using tables of known MZV relations is possible.

Here is a useful proposition giving a condition for determining what the reflective closure of a particular block integral is. This result is visible already in Example 2.2.25.

Proposition 2.2.26. *Let B be a block decomposition. Suppose $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$. Then*

$$\langle B \rangle_{\mathcal{R}} = \left\{ (\epsilon_1;\ \ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \,\middle|\, \sigma \in S_n \right\} .$$

That is, the reflective closure consists of block decompositions arising from all possible permutations of the ℓ_i.

Proof. Since the reflection operators include the operators $\mathcal{R}_{i,i+1}$ which give transpositions $(i, i+1)$ on the ℓ_i, we necessarily generate every permutation of the ℓ_i. But then this set is reflectively closed. Applying $\mathcal{R}j, k$, then merely gives a permutation of the ℓ_i, all of which are already in the set. □

We will need the following lemma in order to compute (or rather disregard) certain subsequences from the calculation of $D_{<n}$.

Lemma 2.2.27. *Suppose that B is the block decomposition of some iterated integral, and further suppose that $\mathcal{R}_{jk} B = B$, for some j, k. Then, in particular, $B^{\mathrm{L}}_{k-i} = B^{\mathrm{L}}_{j+i}$, for $0 \leq i \leq k - j$. Moreover, if $k - j + 1$ is even, or if $k - j + 1$ is odd and $B^{\mathrm{L}}_{j+(k-j)/2}$ is odd, then $B^{\mathrm{st}}_j = B^{\mathrm{en}}_k$.*

Proof. By the definition of $\mathcal{R}_{jk}$ on B, it is clear that $B^{\mathrm{L}}_{j+i} = B^{\mathrm{L}}_{k-i}$ since $B^{\mathrm{L}}_{j+i} = (\mathcal{R}_{jk} B)^{\mathrm{L}}_{j+i} = B^{\mathrm{L}}_{k+j-(j+i)} = B^{\mathrm{L}}_{k-i}$.

By removing blocks $< j$, and removing blocks $> k$, we can assume that the computation is of $\mathcal{R}_{1n} B$, with B having n blocks. The case where $k - j + 1$ is even corresponds to n even, and the case $k - j + 1$ is odd corresponds to n odd.

For $n = 2m$ even, we have that $B^{\mathrm{en}}_m = B^{\mathrm{st}}_{m+1}$ by the definition of a block decomposition. Since $B^{\mathrm{L}}_m = B^{\mathrm{L}}_{m+1}$, we see that $B^{\mathrm{st}}_m = B^{\mathrm{en}}_{m+1}$. Continue this outwards until we get $B^{\mathrm{st}}_1 = B^{\mathrm{en}}_n$.

For $n = 2m + 1$ odd, we have $(\mathcal{R}_{1n} B)^{\mathrm{st}}_{m+1} = B^{\mathrm{st}}_{m+1}$ by assumption. We have that $(j + (k - j)/2)$ corresponds to $1 + (2m + 1 - 1)/2 = m + 1$, so that B^{L}_{m+1} is odd. This means that $B^{\mathrm{en}}_{m+1} = B^{\mathrm{st}}_{m+1} + (B^{\mathrm{L}}_{m+1} - 1) = B^{\mathrm{st}}_{m+1} \pmod 2$. Then use the argument above to work outwards to get $B^{\mathrm{st}}_1 = B^{\mathrm{en}}_n$. □

Example 2.2.28. These examples will illustrate block decompositions which are invariant under some $\mathcal{R}_{j,k}$, and how the start/end point of various blocks behave.

i) For example, the block decomposition $B = (0;\ 3, 4, 4, 3)$ is invariant under $\mathcal{R}_{1,4}$. This corresponds to the word

$$010 \mid 0101 \mid 1010 \mid 010 \,,$$

and indeed $B^{\mathrm{st}}_1 = B^{\mathrm{en}}_4$.

ii) The block decomposition $B = (0;\ 3, 4, 2, 4, 3)$ is invariant under $\mathcal{R}_{1,5}$. This corresponds to the word

$$010 \mid 0101 \mid 10 \mid 0101 \mid 101\,.$$

The middle block has even length, so we do not have $B_1^{\mathrm{st}} = B_5^{\mathrm{en}}$.

iii) However, the block decomposition $B = (0;\ 3, 4, 1, 4, 3)$ is also invariant under $\mathcal{R}_{1,5}$. In this case the middle block has odd length. This corresponds to the word

$$010 \mid 0101 \mid 101 \mid 1010 \mid 010\,,$$

and indeed $B_1^{\mathrm{st}} = B_5^{\mathrm{en}}$.

2.2.4 Reflection operators on subsequences

Using the reflection operators defined above on iterated integrals, we will now define a reflection operator on subsequences marked out on iterated integrals. Using this we can compute D_k, and ultimately prove identities. A special case of this encoding is given in [Cha15], but here we extend the encoding of subsequences to the more general case via the following.

Definition 2.2.29 (Encoding of a subsequence)**.** Suppose w is a word describing some iterated integral $I^{\mathfrak{m}}(w)$, and let P be a subsequence of w of length ≥ 2, in the sense of the derivation's D_r. Then the *encoding of the subsequence* P on w is given by the following data:

- the block encoding $B = \mathrm{block}(w)$ of the word w, upon which P is defined,
- the block s in which P starts,
- the block t in which P finishes,
- the number of letters ℓ before P in the block s, and
- the number of letters m after P in the block t.

We assemble these into the tuple, and identify it with the subsequence to write

$$P = (B; s, t; \ell, m)\,.$$

We may also say that P is a subsequence on the block decomposition B

Observation 2.2.30. From these data, we can calculate the length of the subsequence as $\sum_{i=s}^{t} B_i^{\mathrm{L}} - \ell - m$.

Lemma 2.2.31. *An encoding $(B; s, t; \ell, m)$ of a subsequence is valid (that is, corresponds to a subsequence of length ≥ 2) if and only if the following conditions hold*

i) $1 \leq s \leq t \leq n$, where n is the number of blocks in B, *ii)* $0 \leq \ell < B_s^{\mathrm{L}}$*,*

iii) $0 \leq m < B_t^{\mathrm{L}}$*, and*

iv) if $s = t$*, we must have* $\ell + m + 2 \leq B_s^{\mathrm{L}}$*.*

Proof. The conditions are necessary for the following reasons. Item i) corresponds to the fact that a subsequence starts before it finishes, and lies within the word w. Item ii) corresponds to the fact that the subsequence may start as early as the first letter of a block (so has 0 letters before it), or can start as late as the last letter of the block (so has $B_s^L - 1$ letters before it). Similarly for item iii). Item iv) corresponds to the fact that when a subsequence lies entirely within one block, it must start before it finishes and have length ≥ 2.

Conversely, given a subsequence encoding satisfying these conditions, we can mark uniquely a subsequence on the word $w = \mathrm{word}(B)$ as follows. Find blocks s and t in B; the first condition ensures blocks with these indices exist, and that block s is before block t. Count ℓ letters from the start of block B_s to find the starting point of the subsequence. This is within block s by condition ii). Similarly, count m letters from the end of block B_t to find the ending point of the subsequence. This is within block t by condition iii).

In the case that $s = t$, condition iv) ensures the start point occurs before the end point, and enough room is left for the sequence to have length ≥ 2. In the case $s \neq t$, the start point occurs before the end point because the start *block* occurs before the end *block*. The subsequence necessarily has length ≥ 2 because it consists of at least one point from each of two different blocks. □

We now define the reflection of a subsequence using the reflection operators defined earlier on words and block decompositions.

Definition 2.2.32 (Reflection of a subsequence)**.** Let $P = (B; s, t; \ell, m)$ be a subsequence on some word w with block decomposition B, which describes some iterated integral $I^{\mathfrak{m}}(w)$. Then the reflection operator $\mathcal{R}$ is defined on P by

$$\mathcal{R}P = (\mathcal{R}_{st}B; s, t; m, \ell) \, .$$

One should check that this actually does describe a subsequence on some word. For this we have

Lemma 2.2.33. *On applying the reflection operator* $\mathcal{R}$ *to a subsequence* $P = (B; s, t; \ell, m)$*, we obtain a valid(!) subsequence on the word* $w = \mathrm{word}(\mathcal{R}_{st}B)$*.*

Proof. We need to check the conditions in Lemma 2.2.31 hold. We have that $\mathcal{R}P = (\mathcal{R}_{s,t}B; s, t; m, \ell)$, so the 'subsequence' is defined on $\mathcal{R}_{s,t}B$.

Condition i) requires $1 \leq s \leq t \leq m$, where m is the number of blocks in $\mathcal{R}_{s,t}B$. But since $\mathcal{R}_{s,t}$ preserves the number of blocks by Lemma 2.2.17, $m = n$, where n is the number of blocks in B. Since P is a valid subsequence we know $1 \leq s \leq t \leq n$ holds. So we conclude condition i) holds for $\mathcal{R}P$.

Condition ii) requires $0 \leq m < (\mathcal{R}_{s,t}B)_s^{\mathrm{L}}$. But by definition $(\mathcal{R}_{s,t}B)_s^{\mathrm{L}} = B_{(s+t)-s}^{\mathrm{L}} = B_t^{\mathrm{L}}$. And then $0 \leq m < B_t^{\mathrm{L}}$ holds because it is condition iii) for P.

Similarly iii) requires $0 \leq \ell < (\mathcal{R}_{s,t}B)_t^{\mathrm{L}}$. But $(\mathcal{R}_{s,t}B)_t^{\mathrm{L}} = B_{(s+t)-t}^{\mathrm{L}} = B_s^{\mathrm{L}}$. And then $0 \leq \ell < B_s^{\mathrm{L}}$ holds because it is condition ii) for P.

Lastly condition iv) requires $m + \ell + 2 \leq B_s^{\mathrm{L}}$ if $s = t$. But this condition is exactly the same as condition iv) for P, so it holds.

Therefore $\mathcal{R}P$ defines a valid subsequence on $\mathcal{R}_{st}B$. ☐

Lemma 2.2.34. *The operator $\mathcal{R}$ preserves the length of a subsequence.*

Proof. Let $P = (B; s, t; \ell, m)$ be a subsequence. Then $\mathcal{R}P = (\mathcal{R}_{s,t}B; s, t; m, \ell)$. Using Observation 2.2.30 we compute the length of $\mathcal{R}P$ to be

$$\sum_{i=s}^{t} (\mathcal{R}_{st}B)_i^{\mathrm{L}} - m - \ell = \sum_{i=s}^{t} B_{t+s-i}^{\mathrm{L}} - \ell - m = \sum_{i=s}^{t} B_i^{\mathrm{L}} - \ell - m \,,$$

which is exactly the length of P. ☐

Lemma 2.2.35. *The operator $\mathcal{R}$ is an involution on the set of all subsequences on block decompositions with weight t and n blocks.*

Proof. Let P be a subsequence on some block decomposition B with weight t and n blocks. We have from Lemma 2.2.18, that $\mathcal{R}_{s,t}$ is an involution on this set of iterated integrals, so that $\mathcal{R}_{st}\mathcal{R}_{st}B = B$. Therefore, we compute

$$\begin{aligned} \mathcal{R}\mathcal{R}P &= \mathcal{R}(\mathcal{R}_{st}B; s, t; m, \ell) \\ &= (\mathcal{R}_{st}\mathcal{R}_{st}B; s, t; \ell, m) \\ &= (B; s, t; \ell, m) \\ &= S \,. \end{aligned}$$

☐

Example 2.2.36. Consider the indicated subsequence on the following word.

$$0 \mid 01\,\underbrace{010 \mid 01 \mid 1 \mid 1}\,010101 \mid 10 \mid 01 \mid 1 \,.$$

We know the block decomposition from Example 2.2.9. The encoding of this subsequence is therefore

$$\big((0;\ 1, 5, 2, 1, 7, 2, 2, 1); 2, 5; 2, 6\big) \,.$$

We compute that

$$\begin{aligned} &\mathcal{R}\big((0;\ 1, 5, 2, 1, 7, 2, 2, 1); 2, 5; 2, 6\big) \\ &= \big(\mathcal{R}_{2,5}(0;\ 1, 5, 2, 1, 7, 2, 2, 1); 2, 5; 6, 2\big) \\ &= \big((0;\ 1, 7, 1, 2, 5, 2, 2, 1); 2, 5; 6, 2\big) \,, \end{aligned}$$

using the computation of $\mathcal{R}_{2,5}$ from Example 2.2.19. We therefore obtain the following subsequence on the transformed word

$$0 \mid 010101\underbrace{0 \mid 0 \mid 01 \mid 101}01 \mid 10 \mid 01 \mid 1\,.$$

Here we gather some facts about subsequences and their behaviour under the reflection operator $\mathcal{R}R$, which will be used in the following section to generate identities.

Lemma 2.2.37. *Let $P = (B; s, t; \ell, m)$ be a subsequence. Then as words, the subsequence $\mathcal{R}P$ is either the reverse of P, or the dual of P, i.e. the reverse with $0 \leftrightarrow 1$.*

Proof. By removing the blocks $< s$, and the blocks $> t$, we may assume $s = 1$ and $t = n$, where n is the number of blocks in B.

In the case where $B_1^{\mathrm{st}} = B_n^{\mathrm{en}}$, we will show that the subsequence $\mathcal{R}P$ is the reverse of the subsequence P. Let $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$. The first digit of P is then $\epsilon_1 + \ell$. And $\mathcal{R}_{1n}B = (\epsilon_1;\ \ell_n, \ldots, \ell_1)$, so the last digit of $\mathcal{R}P$ is $(\mathcal{R}_{1n}B)_n^{\mathrm{en}} - \ell$. As in Equation 2.2.1 in the proof of Lemma 2.2.12, we have that $(\mathcal{R}_{1n}B)_n^{\mathrm{en}} = \epsilon_1 + \sum_{i=1}^n (\ell_i - 1) = B_n^{\mathrm{en}} \pmod 2$ and by assumption this is $= B_1^{\mathrm{st}} \pmod 2$. So the last digit of $\mathcal{R}P$ is $B_1^{\mathrm{st}} - \ell$, which equals the first.

We can repeat this one letter at a time to see that the subsequence $\mathcal{R}P$ is exactly the reverse of P.

In the case where $B_1^{\mathrm{st}} \neq B_n^{\mathrm{en}}$, the $\mathcal{R}P$ is the dual of the subsequence P. Observe that in this case we have that the last digit is $1 - B_1^{\mathrm{st}} - \ell$, so at every point we have the extra step of taking $1 - B_i^{\mathrm{en}}$. Not only is the subsequence reversed, but we also interchange $0 \leftrightarrow 1$, giving the dual overall. □

Recall from Definition 1.2.14 that a subsequence (of odd length ≥ 3) is called trivial if the first and last digits are the same. When the first and last digit are the same, the integral of the subsequence is trivially 0 by the equal boundaries property from Property 1.1.13, so it will contribute nothing to $D_{\leq N}$.

Lemma 2.2.38. *Suppose that the subsequence P is a fixed point of the reflection operator $\mathcal{R}$. Further, suppose that P has odd length. Then P is trivial.*

Proof. If $P = (B; s, t; \ell, m)$ is a fixed point, then we must have $\mathcal{R}_{st}B = B$, and $\ell = m$ by the definition of $\mathcal{R}$.

Firstly we show that it is not possible for P to have odd length, be a fixed point, and have $t - s + 1$ even. For if this were the case, by Lemma 2.2.27 we necessarily have $B_{s+i}^{\ell} = B_{t-i}^{\ell}$, and no 'middle block'. This means P has length $\sum_{i=s}^t B_i^{\mathrm{L}} - \ell - m = 2\sum_{i=s}^{s+(t-s)/2} B_i^{\ell} - 2\ell = 0 \pmod 2$.

Therefore we are in the case where $t - s + 1$ is odd. Here we claim that we must have $B_{s+(t-s)/2}^{\ell}$ odd. Otherwise as before, P would have length $\sum_{i=s}^t B_i^{\ell} - \ell - m = 2\sum_{i=s}^{s+(t-s)/2} B_i^{\ell} + B_{s+(t-s)/2} - 2\ell = 0 \pmod 2$.

Now we can apply Lemma 2.2.27 to conclude that $B_s^{\mathrm{st}} = B_t^{\mathrm{en}}$, for the subsequence P. Therefore the first digit of P is $B_s^{\mathrm{st}} + \ell$, whilst the last digit of P is $B_t^{\mathrm{en}} - m = B_s^{\mathrm{st}} - \ell = B_s^{\mathrm{st}} + \ell \pmod 2$. Thus the subsequence is trivial. □

Example 2.2.39. Following on from Example 2.2.28, these examples will illustrate when we can have odd length subsequences which are invariant under $\mathcal{R}$, and illustrate the result that these subsequences are in fact trivial.

i) For example, the subsequence $P = ((0;\ 3,4,4,3);1,4;2,2)$ is invariant under $\mathcal{R}_{1,4}$. It is the following subsequence

$$01\,\underbrace{0 \mid 0101 \mid 1010 \mid 0}\,10\,,$$

but this subsequence has even length $1+4+4+1=10$.

ii) The subsequence $P = ((0;\ 3,4,2,4,3);1,5;2,2)$ is invariant under $\mathcal{R}_{1,5}$. It is the following subsequence

$$01\,\underbrace{0 \mid 0101 \mid 10 \mid 0101 \mid 1}\,01\,.$$

The middle block has even length, so this subsequence has even length $1+4+2+4+1=12$.

iii) However the subsequence $P = ((0;\ 3,4,1,4,3);1,5;2,2)$ is also invariant under $\mathcal{R}_{1,5}$. In this case the middle block has odd length. It is the following subsequence

$$01\,\underbrace{0 \mid 0101 \mid 101 \mid 1010 \mid 0}\,10\,,$$

This subsequence has odd length $1+4+3+4+1=13$, and is indeed trivial. The first and last digits of the subsequence are both 0.

2.3 Identities from reflectively closed sets

We are now in a position to use this framework to prove the main theorem of this chapter, from which we can then produce a lot of new identities on MZV's and iterated integrals. These identities will include some motivic proofs, up to a rational, of some currently conjectural results. We give some auxiliary results first, which will be combined to prove the theorem.

In what follows, let S be a reflectively closed subset of

$$H \coloneqq \{\, B \mid B \text{ is a block decomposition, with weight } t \text{ and } n \text{ blocks} \,\}\,.$$

And let T be the set of all odd length subsequences on the block decompositions in S.

Lemma 2.3.1. *The reflection operator $\mathcal{R}$ defines a map from $T \to T$.*

Proof. Let P be a subsequence in T; then $P = (B; s, t; \ell, m)$ for B a block decomposition in S, and some s, t, ℓ, m. We have that $\mathcal{R}P = (\mathcal{R}_{st}B; s, t; m, \ell)$. But from the assumption, S is reflectively closed, and therefore $\mathcal{R}_{st}B$ is some (possibly different) block decomposition in S. We know from Lemma 2.2.33 that $\mathcal{R}P$ defines a subsequence on $\mathcal{R}_{st}B$. Therefore $\mathcal{R}P \in T$, as required. □

We know from Lemma 2.2.35 that $\mathcal{R}$ is an involution on T, meaning that $\mathcal{R}^2 = \mathrm{id}_T$. We can consider the group $G = \{ \mathrm{id}_T, \mathcal{R} \}$, and its action on the set T of subsequences.

Lemma 2.3.2. *The group $G = \{ \mathrm{id}_T, \mathcal{R} \}$ acts on T.*

Proof. This is clear since G is a group of functions, and the action is function application. The rule for evaluating $(f \circ g)(x)$ as $f(g(x))$ is one of the condition for a group action. That the function id_T is the identity function on T is the other condition for a group action. □

Lemma 2.3.3. *The set T breaks up into orbits of size ≤ 2 under the action of $G = \{ \mathrm{id}_T, \mathcal{R} \}$.*

Proof. By the Orbit-Stabilizer theorem, the size of an orbit under this action divides the size of G, which is 2. □

Lemma 2.3.4. *Let O be an orbit of T under G, which has size 1. Then the subsequence in O is trivial, since it has odd length. (Recall, this means the end points of the subsequence are equal.)*

Proof. Suppose $O = \{ P \}$. Then we must have $\mathcal{R}P = P$, so the subsequence P in O is a fixed point of $\mathcal{R}$. Now, since O has odd length, we know from Lemma 2.2.38 that it is trivial. □

Lemma 2.3.5. *Suppose that O is an orbit of T under G, which has size 2. Then either O contains two trivial subsequences, or it contains two non-trivial subsequences.*

Proof. Suppose that $O = \{ P_1, P_2 \}$, and that $P_1 = (B; s, t; \ell, m)$ is non-trivial. We have therefore that the first digit of P_1, which is $B_s^{\mathrm{st}} + \ell$, and the last digit of P_1, which is $B_t^{\mathrm{en}} - m$, are distinct.

Now compute the first and last digit of $P_2 = (\mathcal{R}_{st}B; s, t; m, \ell)$. In the case where $B_s^{\mathrm{st}} = B_t^{\mathrm{en}}$, we get $(\mathcal{R}_{st}B)_s^{\mathrm{st}} = B_t^{\mathrm{en}}$ and $(\mathcal{R}_{st}B)_t^{\mathrm{en}} = B_t^{\mathrm{st}}$, so that the first and last digits of P_2 are $B_t^{\mathrm{en}} + m = B_t^{\mathrm{en}} - m \pmod 2$, and $B_s^{\mathrm{st}} - \ell = B_s^{\mathrm{st}} + \ell \pmod 2$. These are the same as those of P_1, so are still distinct.

In the case where $B_s^{\mathrm{st}} \neq B_t^{\mathrm{en}}$, we find $(\mathcal{R}_{st}B)_s^{\mathrm{st}} = 1 - B_t^{\mathrm{en}}$ and $(\mathcal{R}_{st}B)_t^{\mathrm{en}} = 1 - B_t^{\mathrm{st}}$, so that the first and last digits of P_2 are $1 - B_t^{\mathrm{en}} + m = 1 + B_t^{\mathrm{en}} - m \pmod 2$, and $1 - B_s^{\mathrm{st}} - \ell = 1 + B_s^{\mathrm{st}} + \ell \pmod 2$. Since these are the opposite of those of P_1, they are also distinct. □

Lemma 2.3.6. *Let O be an orbit of T under G, which consists of two non-trivial subsequences. Then the quotient sequences determined by these subsequences are equal, and the integrals of the subsequences are negatives of each other.*

Proof. Let the two subsequence be $P_1 = (B; s, t; \ell, m)$ and $P_2 = \mathcal{R}P_1 = (\mathcal{R}_{st}B; s, t, m, \ell)$. Say $B = (\epsilon_1;\ \ell_1, \ldots, \ell_n)$. Then for $i < s$ and $i > t$, the blocks of B and $\mathcal{R}_{st}B$ agree, so the quotient sequences agree here. Since P_1 is non-trivial, the first and last letters are different. Suppose P starts with x, then it ends with $1 - x$. Set $\delta = B_s^{\mathrm{st}}$. Then the quotient sequence is

$$W_{\epsilon_1}^{\ell_1} \cdots W_{\epsilon_{s-1}}^{\ell_{s-1}} W_{\delta}^{\ell+1} \oplus W_{1-x}^{m+1} W_{\epsilon_{t+1}}^{\ell_{t+1}} \cdots W_{\epsilon_n}^{\ell_n} .$$

Since $W_\delta^{\ell+1}$ ends with x, and W_{1-x}^{m+1} starts with $1-x$, we have

$$W_\delta^{\ell+1} \oplus W_{1-x}^{m+1} = W_\delta^{\ell+m+2} .$$

So the blocks in B are joined by the word $W_\delta^{\ell+m+2}$.

But for the same reason, the blocks in $\mathcal{R}_{st}B$ are joined by $W_\epsilon^{m+\ell+2}$, where $\epsilon = (\mathcal{R}_{st}B)_s^{\mathrm{st}} = B_s^{\mathrm{st}}$, by the definition of $\mathcal{R}_{st}$. Therefore the quotient sequences Q_1 from P_1 and Q_2 from P_2 are both identical. So we certainly have $I^{\mathfrak{m}}(Q_1) = I^{\mathfrak{m}}(Q_2)$.

Using Lemma 2.2.37, we know that the subsequences P_1 and P_2 are either the reverse, or the dual, of each other. If P_2 is the reverse of P_1, then by the reversal of paths property from Property 1.1.13, we have $I^{\mathfrak{L}}(P_1) = -I^{\mathfrak{L}}(P_2)$ since P_1 and P_2 have odd length. If P_2 is the dual of P_1, then by duality, we also have $I^{\mathfrak{L}}(P_1) = -I^{\mathfrak{L}}(P_2)$, since P_1 and P_2 have odd length. □

Lemma 2.3.7. *Let O be an orbit of T under G. Then the sum of the terms this gives rise to in $D_{<N}$ is 0.*

Proof. If O has size 1, then by Lemma 2.3.4, the subsequence in O is trivial, and the orbit O contributes 0 to $D_{<N}$.

If O has size 2, and the two subsequences it contains are trivial, then the orbit O contributes 0 to $D_{<N}$. Otherwise, by Lemma 2.3.5, the two subsequences P_1 and P_2 in O are non-trivial. But then by Lemma 2.3.6 we have $I^{\mathfrak{L}}(P_1) = -I^{\mathfrak{L}}(P_2)$, and $I^{\mathfrak{m}}(Q_1) = I^{\mathfrak{m}}(Q_2)$, where Q_i is the quotient sequence obtained from P_i. Then the orbit O contributes

$$\begin{aligned}
&I^{\mathfrak{L}}(P_1) \otimes I^{\mathfrak{m}}(Q_1) + I^{\mathfrak{L}}(P_2) \otimes I^{\mathfrak{m}}(Q_2) \\
&= I^{\mathfrak{L}}(P_1) \otimes I^{\mathfrak{m}}(Q_1) - I^{\mathfrak{L}}(P_1) \otimes I^{\mathfrak{m}}(Q_1) \\
&= 0 .
\end{aligned}$$

□

At this point we can state and prove the main theorem of this chapter.

Theorem 2.3.8. *Let S be a reflectively closed set of block decompositions with a fixed weight t, and fixed number of blocks. Then the sum of the corresponding block integrals satisfies the following*

$$\sum\nolimits_{s \in S} I_{\mathrm{bl}}^{\mathfrak{m}}(s) \in \zeta^{\mathfrak{m}}(t)\mathbb{Q} .$$

Proof. The goal is to compute $D_{<N}$, for weight $N = t$ on the sum $\sum_{s\in S} I_{\mathrm{bl}}^{\mathfrak{m}}(s)$. Since the coefficients of all the integrals in the sum are $+1$, the terms of $D_{<N}$ arise exactly from the set of all odd subsequences on the block decompositions in S. Write T for the set of all odd subsequences on S.

By Lemma 2.3.3 we know that the set T breaks up into orbits of size ≤ 2 under the action of the group $\{ \mathrm{id}_T, \mathcal{R} \}$ generated by the reflection operator. From Lemma 2.3.7 we know that all of these orbits contribute 0 to $D_{<N}$.

Therefore $D_{<N} \sum_{s\in S} I^{\mathfrak{m}}_{\mathrm{bl}}(s) = 0$, and by Brown's characterisation of $\ker D_{<N}$, Theorem 1.2.15, we have $\sum_{s\in S} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \in \zeta^{\mathfrak{m}}(t)\mathbb{Q}$, as required. ☐

In particular we have the following corollary, which gives a way to *generate* identities, by finding the reflective closure of the block decompositions associated to some initial set of iterated integrals.

Corollary 2.3.9. *Let* $\widetilde{S} = \{ I^{\mathfrak{m}}(w_i) \}$ *be a set of iterated integrals, with corresponding block decompositions* $S = \{ B_i \}$. *Suppose that* S *consists of block decompositions with a fixed weight* N, *and a fixed number of blocks, but that* S *is not necessarily reflectively closed. Then*

$$\sum_{s\in\langle S\rangle_{\mathcal{R}}} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \in \zeta^{\mathfrak{m}}(N)\mathbb{Q}\,.$$

Proof. The set $\langle S\rangle_{\mathcal{R}}$ is reflectively closed by definition, so this result follows immediately from Theorem 2.3.8. ☐

Remark 2.3.10. By applying the period map from Equation 1.2.1 to Theorem 2.3.8, and Corollary 2.3.9, we obtain analogous results on the level of real numbers for the classical iterated integrals and multiple zeta values.

This corroborates the observation in Example 2.2.25, that starting from the integral $I^{\mathfrak{m}}(01010 \mid 01 \mid 101) = \zeta^{\mathfrak{m}}(2,3,1,2)$ with block decomposition $(0;5,2,3)$, the sum

$$\sum_{s\in S'} I^{\mathfrak{m}}_{\mathrm{bl}}(s)\,,$$

over the reflective closure $S' = \langle(0;5,2,3)\rangle_{\mathcal{R}}$, has period in $\pi^8\mathbb{Q} = \zeta(8)\mathbb{Q}$.

2.4 Examples of identities following from reflective closure

In this section we will collect a number of identities which follow from this construction.

Proposition 2.4.1. *Let*

$$H(t,n) \coloneqq \left\{ B \;\middle|\; B \text{ is a block decomposition, with weight } t \text{ and } n \text{ blocks, and } B_1^{\mathrm{st}} = 0 \right\}\,.$$

Then

$$\sum_{s\in H(t,n)} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \in \zeta^{\mathfrak{m}}(t)\mathbb{Q}\,.$$

And applying the period map shows that

$$\mathrm{per}\left(\sum_{s\in H(t,n)} I^{\mathfrak{m}}_{\mathrm{bl}}(s)\right) \in \zeta(t)\mathbb{Q}\,.$$

Proof. The set $H(t,n)$ is reflectively closed because Lemma 2.2.17 shows that the reflection operators preserve weight and number of blocks. They also preserve B_1^{st}. The result follows from Theorem 2.3.8. ☐

Corollary 2.4.2. *Let*

$$H(t) \coloneqq \left\{ \, B \;\middle|\; B \textit{ is a block decomposition, with weight } t \textit{ and } B_1^{\mathrm{st}} = 0 \, \right\} \, .$$

Then

$$\textstyle\sum_{s \in H(t)} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \in \zeta^{\mathfrak{m}}(t)\mathbb{Q} \, .$$

And applying the period map shows that

$$\operatorname{per}\left(\textstyle\sum_{s \in H(t)} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \right) \in \zeta(t)\mathbb{Q} \, .$$

Proof. Technically, we cannot appeal directly to reflective closure, since the number of blocks is not constant in $H(t)$. However, we can write

$$H(t) = \bigcup_{n=1}^{t+2} H(t, n) \, ,$$

where the union is disjoint. It is clear that any integral has at least one block. An integral of weight t is described by a word of length $t+2$. If this is the word constant word $000\cdots 0$, then at $t+2$ blocks are required (one block for every symbol).

Proposition 2.4.1 shows that $\sum_{s \in H(t,n)} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \in \zeta^{\mathfrak{m}}(t)\mathbb{Q}$. Therefore we have

$$\sum_{s \in H(t)} I^{\mathfrak{m}}_{\mathrm{bl}}(s) = \sum_{n=1}^{t+2} \left(\sum_{s \in H(t,n)} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \right) \in \zeta^{\mathfrak{m}}(t)\mathbb{Q} \, . \qquad \square$$

Remark 2.4.3. In the above proposition, we could (should) also impose the condition that the number of blocks in B is different from t modulo 2. If they are equal, the integrals of such blocks are trivially 0 using Lemma 2.2.12, so $\sum_{s \in H(n,t)} I^{\mathfrak{m}}_{\mathrm{bl}}(s) = 0$ if $n = t \pmod 2$.

A more interesting family of identities is the following. They form the most 'basic' type of identity provable within this framework. These identities will arise when we discuss a generalisation of the cyclic insertion conjecture; they will enable us to make some partial progress towards it.

Theorem 2.4.4 (Symmetric insertion)**.** *Let $n \in \mathbb{Z}_{>0}$, and let $\ell_1, \ldots, \ell_n$ be given. Set $t \coloneqq -2 + \sum_{i=1}^n \ell_i$, to be the weight of the integral block decomposition* $(0;\ \ell_1, \ldots, \ell_n)$*, and assume $t \geq 2$. Then*

$$\sum_{\sigma \in S_n} I^{\mathfrak{m}}_{\mathrm{bl}}(0;\ \ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \in \zeta^{\mathfrak{m}}(t)\mathbb{Q} \, .$$

Proof. Essentially this result is equivalent to Theorem 2.3.8, although we restrict to reflectively closed sets generated by one element, and give the corresponding result explicitly in terms of permutations of the blocks.

From Proposition 2.2.26, we have that

$$S \coloneqq \langle (0;\ \ell_1, \ldots, \ell_n) \rangle_{\mathcal{R}} = \left\{ \, (0;\ \ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \;\middle|\; \sigma \in S_n \, \right\} \, .$$

Since $S = \langle (0;\ \ell_1, \ldots, \ell_n) \rangle_{\mathcal{R}}$ is reflectively closed by definition, we conclude by Theorem 2.3.8, that

$$\sum_{\sigma \in S_n} I^{\mathfrak{m}}_{\mathrm{bl}}(0;\ \ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) = \sum_{s \in S} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \in \zeta^{\mathfrak{m}}(t)\mathbb{Q}\,. \qquad \square$$

Remark 2.4.5. At odd weight, all of the above results are, in fact, trivial. This is because, as discussed in Remark 2.2.16, the reflection operator $\mathcal{R}_{1n}$ acting on a block decomposition B with n blocks returns the block decomposition of the dual integral, up to sign. If t is the weight, the duality relation then shows that $I^{\mathfrak{m}}_{\mathrm{bl}}(\mathcal{R}_{1n}B) = (-1)^t I^{\mathfrak{m}}_{\mathrm{bl}}(B)$. So when summing the integrals of a reflectively closed set of odd weight, the terms merely cancel in pairs.

However, at even weight the results are definitely non-trivial, as we shall later see.

2.4.1 Relations on MZV's

It behooves us to consider what sort of identities these results give us about MZV's. We know that every iterated integral $I^{\mathfrak{m}}(w)$ can be expressed in terms of MZV's, by shuffle-regularising the divergences away, as in Section 1.2.3.1. However, this procedure can obscure much of the structure of the original identity. When can we convert directly back to MZV's?

From Lemma 2.2.14, we know divergent integrals correspond to block decompositions B which start with $B^{\mathrm{L}}_1 = 1$, or end with $B^{\mathrm{L}}_n = 1$. Proposition 2.2.26 shows that a reflectively closed set contains all permutations of the lengths B^{L}_i, so to be guaranteed a convergent integral, we must require $B^{\mathrm{L}}_i > 1$ for all i.

Definition 2.4.6. A block decomposition B (with weight different from number of blocks mod 2) which has $B^{\mathrm{L}}_i > 1$ for all i will be called *always convergent.*

Proposition 2.4.7. *Always convergent block decompositions describe MZV's $z = \zeta^{\mathfrak{m}}(a_1, \ldots, a_k)$ satisfying the following conditions:*

i) each argument a_i is contained in $\{1, 2, 3\}$, and

ii) there is no consecutive pair of arguments $a_i = a_{i+1} = 1$.

Proof. An argument $a_i > 3$ in MZV's corresponds to the substring

$$10^{a_i - 1} = 1\underbrace{00\cdots0}_{\geq 3\text{ symbols}}\,.$$

This corresponds to the following decomposition into blocks

$$10 \mid 0 \mid \cdots \mid 0\,,$$

and so cannot occur because length 1 blocks are forbidden.

Similarly consecutive arguments $a_i = a_{i+1} = 1$ correspond to the following substring

$$\cdots \underbrace{1 \mid 1 \mid 1}_{\geq 3\text{ symbols}} \cdots\,,$$

which cannot occur because length 1 blocks are forbidden. □

Definition 2.4.8. Suppose $\zeta(a_1, \ldots, a_k)$ is an MZV satisfying the two conditions

i) each argument a_i is contained in $\{ 1, 2, 3 \}$, and

ii) there is no consecutive pair of arguments $a_i = a_{i+1} = 1$.

We will call this a *123-MZV*.

Using this, we can prove an identity involving a sum of this type of MZV.

Proposition 2.4.9. *Let*

$$S \coloneqq \{ \text{ 123-MZV's of weight } t \ \} \,.$$

Then

$$\textstyle\sum_{z \in S} (-1)^{\mathrm{dp}(z)} z \in \zeta(t)\mathbb{Q} \,,$$

where dp *is the depth of the MZV.*

Proof. First convert this to a statement of iterated integrals. The factor $(-1)^{\mathrm{dp}(z)}$ disappears when we do this conversion.

These MZV's exactly correspond to always convergent block decompositions of weight t, where the number of blocks is different from the weight modulo 2. Including those where number of blocks = weight (mod 2) will not change the sum, as they contribute trivially 0.

The sum then reads

$$\textstyle\sum_{s \in T} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \,,$$

where $T \coloneqq \left\{ B \;\middle|\; B \text{ is a block decomposition, with weight } t,\, B_1^{\mathrm{st}} = 0, \text{ and all } B_i^{\mathrm{L}} > 1 \ \right\}$

Break this into a disjoint union over sets

$$T(n) \coloneqq \left\{ B \;\middle|\; B \text{ is a block decomposition, with weight } t,\, n \text{ bocks}, B_1^{\mathrm{st}} = 0, \text{ and all } B_i^{\mathrm{L}} > 1 \ \right\} \,,$$

which contain block decompositions with a fixed number of blocks. We see that each of these sets is reflectively closed; the reflection operators permute the lengths, so they do not change whether the lengths are all > 1.

So we conclude by Theorem 2.3.8 that

$$\textstyle\sum_{z \in S} (-1)^{\mathrm{dp}(z)} z = \displaystyle\sum_n \left(\textstyle\sum_{s \in T(n)} I^{\mathfrak{m}}_{\mathrm{bl}}(s) \right) \in \zeta(t)\mathbb{Q} \,.$$ □

Remark 2.4.10. This identity breaks up into smaller sums which involve only permutations of some fixed blocks, using Theorem 2.4.4.

Example 2.4.11. At weight 8, there are 17 such 123-MZV's. We obtain the following sums with the indicated block lengths.

Lengths (10): $$\zeta(2,2,2,2) = \frac{\pi^8}{9!}$$

Lengths $(2,2,6)$: $$\zeta(1,3,2,2) + \zeta(1,2,2,3) + \zeta(2,2,1,3) = \frac{\pi^8}{9!}$$

Lengths $(2,3,5)$: $$-\zeta(3,2,3) + \zeta(2,3,1,2) - \zeta(1,2,1,2,2) + \\ -\zeta(2,3,3) + \zeta(3,1,2,2) - \zeta(1,2,2,1,2) = \frac{2\pi^8}{9!}$$

Lengths $(2,4,4)$: $$\zeta(1,2,3,2) + \zeta(2,1,3,2) + \zeta(2,1,2,3) = \frac{\pi^8}{9!}$$

Lengths $(3,3,4)$: $$\zeta(3,3,2) - \zeta(3,2,1,2) + \zeta(2,1,2,1,2) = \frac{\pi^8}{9!}$$

Lengths $(2,2,2,2,2)$: $$\zeta(1,3,1,3) = \frac{\pi^8}{5 \cdot 9!}$$

Here the weight here is low enough that tables of relations can be used to explicitly evaluate these combinations. Alternatively, one can obtain the rational multiple of $\pi^8/9!$ in each identity by numerically evaluating as in Remark 1.2.16, and finding the rational to sufficiently high precision to be confident in the result.

For the sum in Proposition 2.4.9, over

$$S \coloneqq \{ \text{ 123-MZV's of weight 8 } \}$$

we obtain

$$\sum_{z \in S} (-1)^{\mathrm{dp}(z)} z = \frac{31}{5} \frac{\pi^8}{9!}$$

2.5 The (generalised) cyclic insertion conjecture

In this section, we will introduce a generalisation of the cyclic insertion conjecture proposed by Borwein, Bradley, Broadhurst, and Lisoněk in [BBBL98]. Some shadow of this conjecture can be seen in the evaluations presented in Example 2.4.11 above, specifically in the fact that each sum evaluates to a very precise multiple of $\frac{\pi^8}{9!}$.

The name of this conjecture comes from the first instance conjectured in [BBBL98]. In this instance, blocks of 2's were being inserted cyclically into the arguments of another MZV. Whilst the generalisation does not have this particular quality, it still uses a cyclical shifting and so the name remains apt.

Conjecture 2.5.1 (Generalised cyclic insertion)**.** *Let $B = (0;\ \ell_1, \ldots, \ell_n)$ be a block decomposition of weight t. Let $C_n = \langle (1\ 2\ \cdots\ n) \rangle$ be the cyclic group of order n viewed as a subgroup of S_n, generated by the n-cycle $(1\ 2\ \cdots\ n)$.*

i) If B has even weight, n is odd so that the integrals are not trivially zero, and there does not exist a consecutive pair of lengths $B_i^{\mathrm{L}} = B_{i+1}^{\mathrm{L}} = 1$, then

$$\sum_{\sigma \in C_n} I_{\mathrm{bl}}^{\mathfrak{m}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \overset{?}{=} I_{\mathrm{bl}}^{\mathfrak{m}}(t+2) = (-1)^{t/2} \zeta^{\mathfrak{m}}(\{2\}^{t/2}) \,.$$

And applying the period map would give

$$\sum_{\sigma \in C_n} I_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \overset{?}{=} (-1)^{t/2} \frac{\pi^t}{(t+1)!} \in \pi^t \mathbb{Q} \,.$$

ii) If B has odd weight, n is even so that the integrals are not trivially zero, and there does not exist a consecutive pair of lengths $B_i^{\mathrm{L}} = B_{i+1}^{\mathrm{L}} = 1$, then

$$\sum_{\sigma \in C_n} I_{\mathrm{bl}}^{\mathfrak{m}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \overset{?}{=} I_{\mathrm{bl}}^{\mathfrak{m}}(t+2) = 0 \,,$$

with the same result after applying the period map.

One could paraphrase this conjecture as saying roughly that at a given weight, cyclically symmetrised block integrals have a constant value. The restrictions on the B_i^{L} are necessary, as shown in Remark 2.5.3 below.

Evidence and outlook. In Section 2.8 we present tables of the dimensions of cyclic insertion relations (Conjecture 2.5.1), symmetric insertion relations (Theorem 2.5.4), and other numerically verified block relations. In particular, we tested the cyclic insertion conjecture for every valid block decomposition up to weight 16, plus numerous other examples in higher weight.

It appears that the identities in Conjecture 2.5.1 satisfy some sort of 'stability' under the derivations $D_{<N}$, which opens up a potential avenue to a partial 'proof by recursion' using the motivic framework. For further details, see the later Remark 2.6.18 where we can explicitly refer to examples that illustrate this stability. Be aware though, that the motivic framework cannot yet provide a full proof of these results, since the rational multiple needs to be numerically evaluated. □

Remark 2.5.2. Briefly revisiting Example 2.4.11, we should look at the block decompositions with lengths $(2,3,5)$ and $(2,2,2,2,2)$ in a little more detail, just to clarify some points of potential confusion.

The lengths $(2,3,5)$ give rise to the following sum

$$\begin{aligned} &-\zeta(3,2,3) + \zeta(2,3,1,2) - \zeta(1,2,1,2,2) + \\ &- \zeta(2,3,3) + \zeta(3,1,2,2) - \zeta(1,2,2,1,2) = \frac{2\pi^8}{9!} \,. \end{aligned}$$

Each row of this is itself an instance of the cyclic insertion conjecture. The first row cyclically sums over $(2,3,5)$, whilst the second row cyclically sums over $(2,5,3)$. Each row sums to $\frac{\pi^8}{9!}$ according to the cyclic insertion conjecture, explaining the coefficient 2 in the result.

Whereas, for the lengths $(2,2,2,2,2)$, the cyclic insertion conjecture produces 5 copies of the blocks $I^{\mathfrak{m}}_{\mathrm{bl}}(2,2,2,2,2)$ because the blocks are already cyclically symmetric. So we get

$$5I^{\mathfrak{m}}_{\mathrm{bl}}(2,2,2,2,2) \overset{?}{=} I_{\mathrm{bl}}(10) \text{ or}$$
$$5I^{\mathfrak{m}}(0;1,1,0,0,1,1,0,0;1) \overset{?}{=} I^{\mathfrak{m}}(0;1,0,1,0,1,0,1,0;1)\,.$$

Converting to MZV's and applying the period map gives

$$5\zeta(1,3,1,3) = \zeta(2,2,2,2) = \frac{\pi^8}{9!}\,,$$

we can then divide through by 5, to get the result in Example 2.4.11, which explains the coefficient $\frac{1}{5}$.

Remark 2.5.3. The restrictions that there is no pair $B^{\mathrm{L}}_i = B^{\mathrm{L}}_{i+1}$ in both cases, seems somewhat ad-hoc. It appears that these (conjectural) identities are just an easy version of some statement which holds even more generally. These restrictions are most certainly necessary, as shown by the following examples.

In even weight, applying the cyclic insertion conjecture to the blocks $[\ell_i] = [1,1,2,3,3]$ does not produce even a rational multiple of π^8, despite this block decomposition having weight 8. In this case we obtain

$$\sum_{\sigma\in C_5} I_{\mathrm{bl}}(\ell_{\sigma(1)},\ldots,\ell_{\sigma(5)}) = 27.89973142\ldots\frac{\pi^8}{9!}\,.$$

However, we do obtain (by use of Theorem 2.5.4 below) that the fully symmetrised sum does produce a rational multiple of π^8, namely

$$\sum_{\sigma\in S_5} I_{\mathrm{bl}}(\ell_{\sigma(1)},\ldots,\ell_{\sigma(5)}) = -18\frac{\pi^8}{9!} \in \pi^8\mathbb{Q}\,.$$

Similarly, in the odd weight case, applying the cyclic insertion conjecture to the blocks $[\ell_i] = [1,1,2,3]$ produces a non-zero result in contrast to the result of 0 we would desire. Specifically

$$\begin{aligned}\sum_{\sigma\in C_4} I_{\mathrm{bl}}(\ell_{\sigma(1)},\ldots,\ell_{\sigma(4)}) &= 3.95460870059\ldots\\ &= 2\zeta(2)\zeta(3)\,.\end{aligned}$$

In the context of Remark 2.6.18, this cyclic combination for $[\ell_i] = [1,1,2,3]$ appears as part of the computation of D_3 for the cyclic combination $[\ell_i] = [1,1,2,3,3]$ above. This in fact leads to the result that for $[\ell_i] = [1,1,2,3,3]$,

$$\sum_{\sigma\in C_5} I_{\mathrm{bl}}(\ell_{\sigma(1)},\ldots,\ell_{\sigma(5)}) = \zeta(2)\zeta(3)^2 - 63\frac{\pi^8}{9!}\,.$$

Alternatively (after applying some identities), this may be written as

$$\begin{aligned}&= 2\zeta(2)\zeta(1,2,1,2) + \zeta(2,2,2,2,2)\\ &= -2I_{\mathrm{bl}}(4)I_{\mathrm{bl}}(2,3,3) + I_{\mathrm{bl}}(10)\,,\end{aligned}$$

where the blocks $[2,3,3]$ from $[\ell_i]$ make a second appearance.

This indeed offers a suggestion for how to generalise the cyclic insertion conjecture to all block decompositions. From recent cursory investigations, it appears a general result holds for $[\ell_i] = [k_1, \ldots, k_{n-2}, 1, 1]$, where $k_1 \neq 1$, $k_{n-2} \neq 1$, and there is no pair $k_i = k_{i+1} = 1$. The result is as follows.

$$\sum_{\sigma \in C_n} I_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \overset{?}{=} -2 I_{\mathrm{bl}}(4) I_{\mathrm{bl}}(k_1, \ldots, k_n) + I_{\mathrm{bl}}(k_1 + \cdots + k_{n-2} + 2) \, .$$

Generalisations to $[\ell_i] = [k_1, \ldots, k_{n-3}, 1, 1, 1]$ and beyond also appear to hold.

We claim now that the generalised cyclic insertion conjecture (Conjecture 2.5.1) is a generalisation of both the BBBL cyclic insertion conjecture, and of Hoffman's identity. This will be shown explicitly in Conjecture-Example 2.6.1 and Conjecture-Example 2.6.4. It is not surprising then that we cannot prove this conjecture. We can make some progress towards it in the form of the following theorem, which is a restatement and reinterpretation of Theorem 2.4.4 applied to the context of Conjecture 2.5.1.

Theorem 2.5.4 (Generalised symmetric insertion)**.** *Let $B = (0;\ \ell_1, \ldots, \ell_n)$ be a block decomposition of even weight t. Then some sufficiently symmetrised version of Conjecture 2.5.1 holds. More precisely the following evaluation, consisting of a sum of $(n-1)!$ cyclic insertion identities, holds*

$$\sum_{\sigma \in S_n} I^{\mathfrak{m}}_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \in \zeta^{\mathfrak{m}}(\{2\}^{t/2})\mathbb{Q} = \zeta^{\mathfrak{m}}(t)\mathbb{Q} \, .$$

So applying the period map produces

$$\sum_{\sigma \in S_n} I_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) \in \zeta(\{2\}^{t/2})\mathbb{Q} = \zeta(t)\mathbb{Q} = \pi^t \mathbb{Q} \, .$$

Proof. This result is a restatement and reinterpretation of Theorem 2.4.4. The equalities follow using the evaluations (and their motivic counterparts) which state

$$\begin{aligned} \zeta(\{2\}^k) &= \frac{\pi^{2k}}{(2k+1)!} \\ \zeta(2k) &= \frac{(-1)^{k+1} B_{2k} (2\pi)^{2k}}{2(2k)!} \, . \end{aligned}$$

The result holds in fact for any choice of ℓ_i, including in the case where some consecutive pair $\ell_i = \ell_{i+1} = 1$ occurs. □

Remark 2.5.5. An analogous result for odd weight does hold, but is trivial. The symmetrisation produced by Theorem 2.4.4 cancels pairwise, an integral with its dual, to give 0.

In the following section we will present a number of examples of conjectural identities given by the cyclic insertion conjecture, Conjecture 2.5.1, along with the proven symmetrisations from Theorem 2.5.4. Typically we will restrict these examples to 123-MZV's, since they produce 'nice' identities, so I am content to give two simple examples of the general case of cyclic insertion here.

Example 2.5.6. Consider the MZV $z = -\zeta(4,1,2)$, which corresponds to the integral $I(010 \mid 0 \mid 01 \mid 101)$, with block decomposition $I_{\mathrm{bl}}(3,1,2,3)$.

Taking $[\ell_1, \ell_2, \ell_3, \ell_4] = [3,1,2,3]$, we form the sum

$$\begin{aligned}
&\sum_{\sigma \in C_4} I_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(4)}) \\
&= I_{\mathrm{bl}}(3,1,2,3) + I_{\mathrm{bl}}(1,2,3,3) + I_{\mathrm{bl}}(2,3,3,1) + I_{\mathrm{bl}}(3,3,1,2) \\
&= I(010 \mid 0 \mid 01 \mid 101) + I(0 \mid 01 \mid 101 \mid 101) + \\
&\quad + I(01 \mid 101 \mid 101 \mid 1) + I(010 \mid 010 \mid 0 \mid 01)\,.
\end{aligned}$$

The first and last integrals can be converted directly to the MZV's $-\zeta(4,1,2)$ and $\zeta(3,4)$ respectively. The second and third require shuffle-regularising, as in Section 1.2.3.1. They give the following

$$\begin{aligned}
I(001101101) &= -I(010101101) - 2I(011001101) - I(011010101) - 2I(011011001) \\
&= -\zeta(2,2,1,2) - 2\zeta(1,3,1,2) - \zeta(1,2,2,2) - 2\zeta(1,2,1,3) \\
I(011011011) &= 3I(010001001) + 3I(010010001) \\
&= 3\zeta(4,3) + 3\zeta(3,4)\,.
\end{aligned}$$

Thus we obtain the sum

$$\begin{aligned}
\sum_{\sigma \in C_4} I_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(4)}) &= (-\zeta(4,1,2)) + (\zeta(3,4)) + (3\zeta(4,3) + 3\zeta(3,4)) + \\
&\quad + (-\zeta(2,2,1,2) - 2\zeta(1,3,1,2) - \zeta(1,2,2,2) - 2\zeta(1,2,1,3))\,,
\end{aligned}$$

which indeed equals 0, using tables of known MZV relations. This is the result expected by cyclic insertion.

Example 2.5.7. Consider the MZV $z = -\zeta(1,1,2,2,4)$, which corresponds to the integral $I(01 \mid 1 \mid 101010 \mid 0 \mid 01)$, with block decomposition $I_{\mathrm{bl}}(2,1,6,1,2)$.

Take $[\ell_i] = [2,1,6,1,2]$, and form the sum

$$\sum_{\sigma \in C_5} I_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(5)})\,.$$

We obtain

$$\begin{aligned}
&I_{\mathrm{bl}}(2,1,6,1,2) + I_{\mathrm{bl}}(1,6,1,2,2) + I_{\mathrm{bl}}(6,1,2,2,1) + I_{\mathrm{bl}}(1,2,2,1,6) + I_{\mathrm{bl}}(2,2,1,6,1) \\
&= I(01 \mid 1 \mid 101010 \mid 0 \mid 01) + I(0 \mid 010101 \mid 1 \mid 10 \mid 01) + I(010101 \mid 1 \mid 10 \mid 01 \mid 1) + \\
&\quad + I(0 \mid 01 \mid 10 \mid 0 \mid 010101) + I(01 \mid 10 \mid 0 \mid 010101 \mid 1)
\end{aligned}$$

These integrals shuffle regularise to give the following sum of MZV's, where some terms have been combined via duality. The first integral gives the first term. The second and fifth integrals give the third term. And the third and fourth integrals give the second term.

$$\begin{aligned} = & -\zeta(1,1,2,2,4) + \\ & + 2\cdot(-2\zeta(1,4,2,3) - 2\zeta(1,4,3,2) - 4\zeta(1,5,2,2) - \zeta(2,4,2,2)) + \\ & + 2\cdot(3\zeta(2,2,1,1,4) + \zeta(2,2,1,2,3) + \zeta(2,2,2,1,3) + \\ & \quad + 2\zeta(2,3,1,1,3) + 2\zeta(3,2,1,1,3)) = -\frac{\pi^{10}}{11!}\,. \end{aligned}$$

This evaluation is obtained using tables of known MZV relations. This is indeed the result expected by cyclic insertion.

2.5.1 Cyclic insertion on 123-MZV's

If we restrict to the class of 123-MZV, the associated block decomposition never contains a block of length 1. So any cyclic permutation of the block lengths is guaranteed to produce a convergent integral. This means that the terms produced by the cyclic insertion conjecture can be converted directly to MZV's, and will produce relatively short and highly structured conjectural identities. It is worth considering, then, how these terms can be generated directly from an initial MZV without going through the block decomposition first.

Lemma 2.5.8. *The arguments of a 123-MZV are composed of an arbitrary string formed by concatenating a unique combination of substrings of the following type*

i) $\{2\}^\ell, 3$*, where* $\ell \geq 0$*. This contributes 1 block.*

ii) $\{2\}^\ell, 1, \{2\}^n, 3$*, where* $\ell, n \geq 0$*. This contributes 2 blocks.*

iii) $\{2\}^\ell, \underbrace{(1,2), \{2\}^{m_1}, \ldots, (1,2), \{2\}^{m_k}}_{k\text{ repetitions}}, 1, \{2\}^n, 3$*, where* $\ell, m_i, n \geq 0$*. This contributes* $k+2$ *blocks.*

Then ending with

iv) $\{2\}^\ell$*, where* $\ell \geq 0$*. This contributes* 1 *block.*

v) $\{2\}^\ell, \underbrace{(1,2), \{2\}^{m_1}, \ldots, (1,2), \{2\}^{m_k}}_{k\text{ repetitions}}$*, where* $\ell, m_i \geq 0$*. This contributes* $k+1$ *blocks.*

Here the notation $(1,2)$ *is just to emphasise that in these MZV's* $(1,2)$ *seems to function as one argument. One should perhaps view it as* $\overline{3}$*, the dual of* 3.

Proof. In the block decomposition, consider the position of the first block after B_1 which has $B_i^{\mathrm{st}} = 0$. Suppose this block occurs at position $i = 2$, the first such available position. Since the first block must end 0 to make $B_2^{\mathrm{st}} = 0$, the first block must have odd length. Since we restrict to 123-MZV's, all lengths must be > 1. So the word in the integral representation of the MZV must begin

$$0(10)^\ell 10 \mid 0 \cdots = W_0^{2\ell+3} \oplus \cdots\,,$$

where $\ell \geq 0$. This gives case i).

Now suppose the block occurs at position $i > 2$. Then the first block must end 1, meaning it has even length. The blocks in position $j = 2, \ldots, i-2$ must start 1 and end 1, giving them odd length. Finally the block in position $i-1$ must end 0, giving it even length. Restricting to 123-MZV's forces all lengths to be > 1. So the word in the integral representation of the MZV must begin

$$\begin{aligned} &0(10)^\ell 1 \mid 10(10)^{m_1} 1 \mid \cdots \mid 10(10)^{m_k} 1 \mid 10(10)^n \mid 0 \cdots \\ &= W_0^{2\ell+2} W_1^{2m_1+3} \cdots W_1^{2m_k+3} W_1^{2n+2} \oplus \cdots \,, \end{aligned}$$

where $\ell, m_1, \ldots, m_k, n \geq 0$. This gives case ii) and iii).

After dealing with all such blocks, there will be blocks with $B_i^{\mathrm{st}} = 0$ remaining. Then the word in the integral representation of the MZV must look as follows

$$0(10)^\ell 1 \mid 10(10)^{m_1} 1 \mid \cdots \mid 10(10)^{m_k} 1 \,,$$

where $\ell, m_i \geq 0$. The first block cannot end with 0, otherwise the second block starts with 0. Similarly all subsequence blocks must end with 1. Since they also start with 1, this forces their lengths to be odd. Finally restricting to 123-MZV's means that all block lengths are > 1. This gives case iv) and v) since no further blocks can occur. □

Notation 2.5.9. It is convenient to separate the blocks of 2's from the surrounding arguments above, and write

$$\zeta(a_1, \ldots, a_k \mid b_1, \ldots, b_k, b_{k+1}) \coloneqq \zeta(\{2\}^{b_1}, a_1, \{2\}^{b_2}, a_2, \ldots, \{2\}^{b_k}, a_k, \{2\}^{b_{k+1}}) \,,$$

where $a_i \in \{ 1, 3, (1,2) \}$. The substrings in Lemma 2.5.8 forbid consecutive arguments $a_i = (1,2)$ and $a_{i+1} = 3$. This will consist of $k+1$ blocks.

Definition 2.5.10 (Cyclic operator)**.** Let $z = \pm\zeta(a_1, \ldots, a_k \mid b_1, \ldots, b_{k+1})$ be a 123-MZV with corresponding block decomposition $I_{\mathrm{bl}}(\ell_1, \ldots, \ell_n)$, where $n = k+1$. Assume the sign is chosen so that we have equality. Let i be the first position for which $B_i^{\mathrm{st}} = 0$, not including B_1. Define

$$\mathcal{C} z = w \,,$$

where w is the 123-MZV with block decomposition

$$I_{\mathrm{bl}}(\ell_i, \ell_{i+1}, \ldots, \ell_n, \ell_1, \ldots, \ell_{i-1}) \,.$$

If no such i exists, set

$$\mathcal{C} z = w$$

where w is the 123-MZV with block decomposition

$$I_{\mathrm{bl}}(\ell_2, \ell_3, \ldots, \ell_n, \ell_1)$$

Proposition 2.5.11. *Let $\pm\zeta(a_1, \ldots, a_k \mid b_1, \ldots, b_{k+1})$ be a 123-MZV with corresponding block decomposition $I_{\mathrm{bl}}(\ell_1, \ldots, \ell_n)$, where $n = k+1$. Assume the sign is chosen so that we have equality. Then the set*

$$\{\, \mathcal{C}^i z \mid i = 0, \ldots, n-1 \,\}$$

contains exactly the same terms as produced by sum $\sum_{C_n} I_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)})$, from the cyclic insertion conjecture.

That is

$$\sum_{\sigma \in C_n} I_{\mathrm{bl}}(\ell_{\sigma(1)}, \ldots, \ell_{\sigma(n)}) = \sum_{i=0}^{n-1} \mathcal{C}^i z \,.$$

Proof. From the definition it is clear that each term is one of the terms from the cyclic insertion conjecture. Namely, each application of $\mathcal{C}$ produces a cyclic shifting of the block decomposition. We only have to show that eventually any ℓ_i is moved to the first position.

Let $S = \{\, i > 1 \mid B_i^{\mathrm{st}} = 0 \,\}$, and $T = \{\, i > 1 \mid B_i^{\mathrm{st}} = 1 \,\}$. The block corresponding to the j-th element of S is moved to position one by applying $\mathcal{C}^j$. Application of $\mathcal{C}$ changes the starting digit of the blocks $\ell_1, \ldots, \ell_i$ which are moved to the end. This is because the starting digit of $B_1^{\mathrm{st}} = 0$ must be flipped to match the last digit $B_n^{\mathrm{en}} = 1$. Therefore the block corresponding to the j-th element of T is moved to position one by applying $\mathcal{C}^{|S|+j}$. ☐

Proposition 2.5.12. *Let $\zeta(a_1, \ldots, a_k \mid b_1, \ldots, b_{k+1})$ be a 123-MZV. In accordance with the cases in Lemma 2.5.8, application of the cyclic operator $\mathcal{C}$ has the following results.*

i) $\zeta(3, \mathrm{rest} \mid \ell, \mathrm{rest}) \mapsto -\zeta(\mathrm{rest}, (1,2) \mid \mathrm{rest}, \ell)$,

ii) $\zeta(1, 3, \mathrm{rest} \mid \ell, n, \mathrm{rest}) \mapsto \zeta(\mathrm{rest}, 1, 3 \mid \mathrm{rest}, \ell, n)$ *and*

iii) $\zeta(\{(1,2)\}^k, 1, 3, \mathrm{rest} \mid \ell, m_1, \ldots, m_k, n, \mathrm{rest}) \mapsto$
$(-1)^k \zeta(\mathrm{rest}, 1, 3, \{3\}^k \mid \mathrm{rest}, \ell, m_1, \ldots, m_k, n)\,.$

Otherwise, only the final substrings appear, and we have

iv) $\zeta(\emptyset \mid \ell) \mapsto \zeta(\emptyset \mid \ell)$,

v) $\zeta(\{(1,2)\}^k \mid \ell, m_1, \ldots, m_k) \mapsto \zeta(\{3\}^k \mid m_1, \ldots, m_k, \ell)$.

Proof. The proof of Lemma 2.5.8 made use of the position of the first block beginning $B_i^{\mathrm{st}} = 0$. So $\mathcal{C}$ interacts well with the structure presented there. So we can check on a case by case basis.

Case i): The word describing the integral corresponding to the MZV starts

$$0(10)^\ell 10 \mid 0 \cdots = W_0^{2\ell+3} \oplus \cdots \,.$$

So only the first block is moved in this case. The 0 at the start of the second block becomes the lower bound of the integral, so the arguments after $\{2\}^\ell, 3$ will remain unchanged. Moving this block to the end, we obtain

$$\cdots 1 \mid 1(01)^\ell 01 = \cdots \oplus W_1^{2\ell+3} .$$

The upper bound of the integral now becomes the start of the next argument at the end of the MZV. This gives new arguments

$$(1,2), \{2\}^\ell$$

at the end. The depth changes by one, 3 becoming $(1,2)$, so we pick up a minus sign when converting from the integral back to an MZV.

Case ii) and iii): The word describing the integral starts

$$\begin{aligned} &0(10)^\ell 1 \mid 10(10)^{m_1} 1 \mid \cdots \mid 10(10)^{m_k} 1 \mid 10(10)^n \mid 0 \cdots \\ &= W_0^{2\ell+2} W_1^{2m_1+3} \cdots W_1^{2m_k+3} W_1^{2n+2} \oplus \cdots . \end{aligned}$$

In this case the first $k+2$ blocks are moved. The 0 at the start of the $(k+3)$-th block becomes the lower bound of the integral, so the arguments after our initial string will remain unchanged. Moving these blocks to the end gives

$$\begin{aligned} &\cdots 1 \mid 1(01)^\ell 0 \mid 01(01)^{m_1} 0 \mid \cdots \mid 01(01)^{m_k} 0 \mid 01(01)^n \\ &= \cdots \oplus W_1^{2\ell+2} W_0^{2m_1+3} \cdots W_0^{2m_k+3} W_0^{2n+2} \oplus \cdots . \end{aligned}$$

The upper bound of the integral now becomes the start of the next argument at the end of the MZV. This gives new arguments

$$1, \{2\}^\ell, 3, \{2\}^{m_1}, 3, \ldots, \{2\}^{m_k}, 3, \{2\}^n$$

at the end. The depth changes by k, as k arguments of the form $(1,2)$ become arguments of the form 3. So we pick up sign $(-1)^k$ when converting from the integral back to an MZV.

Case iv) and v): The word describing the integral is

$$0(10)^\ell 1 \mid 10(10)^{m_1} 1 \mid \cdots \mid 10(10)^{m_k} 1 = W_0^{2\ell+2} W_1^{2m_1+3} \cdots W_1^{2m_k+3} .$$

By definition, we only move one block to the end in this case. We obtain

$$01(01)^{m_1} 0 \mid \cdots \mid 01(01)^{m_k} 0 \mid 0(10)^\ell 1 = W_0^{2m_1+3} \cdots W_0^{2m_k+3} W_1^{2\ell+2} .$$

This gives the MZV

$$(-1)^k \zeta(\{2\}^{m_1}, 3, \ldots, \{2\}^{m_k}, 3, \{2\}^\ell) .$$

The depth changes by k since k arguments $(1,2)$ become arguments 3. So we pick up a sign $(-1)^k$. □

We will give examples of this proposition in action in the following section, where we present various examples of cyclic insertion and symmetric insertion.

2.6 Examples of cyclic insertion, and symmetrisations

In this section, we will present various examples of the kind of identities one can obtain from cyclic insertion. We will also present the motivically provable symmetrisations which give currently best known identities in that direction. We will at last show how the BBBL cyclic insertion conjecture, and Hoffman's identity, arise from the general conjecture.

Conjecture-Example 2.6.1 (BBBL cyclic insertion)**.** Consider

$$\begin{aligned} z &= (-1)^d \zeta(\{2\}^{a_1}, 1, \{2\}^{a_2}, 3, \{2\}^{a_3}, \ldots, 1, \{2\}^{a_{2n}}, 3, \{2\}^{a_{2n+1}}) \\ &= (-1)^d \zeta(\{1,3\}^n \mid a_1, \ldots, a_{2n+1}) \,, \end{aligned}$$

where $d = 2n + \sum_i a_i$ is the depth, so that the corresponding integral has coefficient 1. Applying the cyclic operator $\mathcal{C}$ produces

$$\begin{aligned} \mathcal{C}z &= (-1)^d \mathcal{C}\zeta(1, 3, \{1,3\}^{n-1} \mid a_1, a_2, a_3, \ldots, a_n) \\ &= (-1)^d \zeta(\{1,3\}^{n-1}, 1, 3 \mid a_3, \ldots, a_n, a_1, a_2) \\ &= (-1)^d \zeta(\{1,3\}^n \mid a_3, \ldots, a_n, a_1, a_2) \,. \end{aligned}$$

That is, the blocks of two $\{2\}^{a_i}$ are cycled around by two steps.

One finds that the integral describing z has $2n+1$ blocks, namely

$$\begin{aligned} z &= I(0(10)^{a_1}1 \mid 10(10)^{a_2} \mid \cdots \mid 0(10)^{a_{2n+1}}1) \\ &= I_{\mathrm{bl}}(2a_1 + 2, 2a_2 + 2, \ldots, 2a_{2n+1} + 2) \,. \end{aligned} \tag{2.6.1}$$

Since there are an odd number of blocks of 2, we conclude that

$$\sum_{i=0}^{n} \mathcal{C}^i z = (-1)^d \sum_{\sigma \in C_{2n+1}} \zeta(\{1,3\}^n \mid a_{\sigma(1)}, \ldots, a_{\sigma(2n+1)}) \,.$$

From Proposition 2.5.11, we know this matches with the sum in the general cyclic insertion conjecture Conjecture 2.5.1. Then that conjecture tells us to expect

$$(-1)^d \sum_{\sigma \in C_{2n+1}} \zeta(\{1,3\}^n \mid a_{\sigma(1)}, \ldots, a_{\sigma(2n+1)}) \overset{?}{=} (-1)^{t/2} \frac{\pi^t}{(t+1)!} \,,$$

as the weight $t = 4n + 2\sum a_i$, even. Since $(-1)^{t/2} = (-1)^{2n + \sum_i a_i} = (-1)^d$, the sign on the RHS matches the sign on the LHS. Therefore we can write wt for the weight, and simplify this to

$$\sum_{\sigma \in C_{2n+1}} \zeta(\{1,3\}^n \mid a_{\sigma(1)}, \ldots, a_{\sigma(2n+1)}) \overset{?}{=} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!} \,.$$

This is exactly the statement of the BBBL cyclic insertion conjecture from Conjecture 2.1.5.

Theorem 2.6.2 (Symmetrised BBBL, [Cha15])**.** *Theorem 2.5.4 shows the following symmetrisation of Conjecture-Example 2.6.1 holds.*

$$\sum_{\sigma \in S_{2n+1}} \zeta(\{1,3\}^n \mid a_{\sigma(1)}, \ldots, a_{\sigma(2n+1)}) \in \pi^{\mathrm{wt}} \mathbb{Q} \,.$$

This is Theorem 3.1 in [Cha15].

Moreover, we have

$$\sum_{\sigma \in S_{2n+1}} \zeta(\{1,3\}^n \mid a_{\sigma(1)}, \ldots, a_{\sigma(2n+1)}) \overset{1}{=} (2n)! \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!} \,.$$

Here $\overset{1}{=}$ *denotes an identity which holds up to* $\mathbb{Q}$*, and where the expected rational is* 1*. (See Appendix A)*

Proof. To obtain the symmetrisation, Theorem 2.5.4 tell us to replace $\sum_{\sigma \in C_{2n+1}}$ with $\sum_{\sigma \in S_{2n+1}}$. Doing this in the above case we obtain

$$\sum_{\sigma \in S_{2n+1}} I_{\mathrm{bl}}(2a_{\sigma(1)} + 2, 2a_{\sigma(2)} + 2, \ldots, 2a_{\sigma(2n+1)} + 2) \,.$$

Using Equation 2.6.1, we can convert this to

$$\pm \sum_{\sigma \in S_{2n+1}} \zeta(\{1,3\}^n \mid a_{\sigma(1)}, \ldots, a_{\sigma(2n+1)}) \,.$$

But Theorem 2.5.4 shows us

$$\pm \sum_{\sigma \in S_{2n+1}} \zeta(\{1,3\}^n \mid a_{\sigma(1)}, \ldots, a_{\sigma(2n+1)}) \in \zeta(t) \mathbb{Q} \,,$$

where the weight $t = 4n + 2\sum_i a_i$ is even. Since $\pm$ does not change rationality, we get

$$\sum_{\sigma \in S_{2n+1}} \zeta(\{1,3\}^n \mid a_{\sigma(1)}, \ldots, a_{\sigma(2n+1)}) \in \pi^{\mathrm{wt}} \mathbb{Q} \,,$$

as claimed.

Moreover, this is made up of $(2n+1)!/(2n+1) = (2n)!$ cyclic insertion identities, each of which conjecturally contribute one lot of $\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$. Adding these gives the expected identity above. □

By setting $a_1 = a_2 = \cdots = a_{2n+1} = m$ above, we obtain $2n+1$ copies of the same MZV. Dividing through by $2n+1$ we obtain the following corollary which partially confirms Conjecture 2.1.8.

Corollary 2.6.3 (Evaluable family of MZV's)**.** *The following result holds*

$$\zeta(\{\{2\}^m, 1, \{2\}^m, 3\}^n, \{2\}^m) \overset{1}{=} \frac{1}{2n+1} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!} \,,$$

so at least is $\in \pi^{\mathrm{wt}} \mathbb{Q}$*.*

Let us consider how Hoffman's identity fits into this picture. We have the following more general version.

Conjecture-Example 2.6.4 (Hoffman's identity)**.** Consider

$$z = (-1)^d \zeta(\{2\}^a, 3, \{2\}^b, 3, \{2\}^c) = (-1)\zeta(3, 3, \mid a, b, c)\,.$$

Where $d = 2 + a + b + c$ is the depth. This has 3 blocks, and one can check it has block decomposition

$$z = I(0(10)^a 10 \mid 0(10)^b 10 \mid 0(10)^c 1) = I_{\mathrm{bl}}(2a+3, 2b+3, 2c+2)\,. \tag{2.6.2}$$

Applying $\mathcal{C}$ gives

$$\mathcal{C}z = -(-1)^d \zeta(3, (1,2) \mid b, c, a) = I_{\mathrm{bl}}(2b+3, 2c+2, 2a+3) \tag{2.6.3}$$

$$\mathcal{C}^2 z = (-1)^d \zeta((1,2), (1,2) \mid c, a, b) = I_{\mathrm{bl}}(2c+2, 2a+3, 2b+3)\,. \tag{2.6.4}$$

So from Proposition 2.5.11 and Conjecture 2.5.1 we expect

$$(-1)^d (\zeta(3, 3 \mid a, b, c) - \zeta(3, (1,2) \mid b, c, a) + \zeta((1,2), (1,2) \mid c, a, b)) \overset{?}{=} (-1)^{t/2} \frac{\pi^t}{(t+1)!}\,,$$

as the weight $t = 6 + 2(a+b+c)$ is even. Since $(-1)^{t/2} = (-1)^{3+a+b+c} = -(-1)^d$, we obtain

$$\zeta(3, 3 \mid a, b, c) - \zeta(3, (1,2) \mid b, c, a) + \zeta((1,2), (1,2) \mid c, a, b) \overset{?}{=} -\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.$$

In particular, the case $a = b = 0$ produces Hoffman's original conjectural family, as given in Conjecture 2.1.9.

Theorem 2.6.5 ((Symmetrised) Hoffman's identity)**.** *Symmetrising Hoffman's conjectural identity Conjecture-Example 2.6.4 using Theorem 2.5.4 shows that the following identity holds*

$$\begin{aligned}&\zeta(3, 3, \mid a, b, c) - \zeta(3, (1,2) \mid b, c, a) + \zeta((1,2), (1,2) \mid c, a, b) + \\ &+ \zeta(3, 3, \mid b, a, c) - \zeta(3, (1,2) \mid a, c, b) + \zeta((1,2), (1,2) \mid c, b, a) \overset{1}{=} -2\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.\end{aligned}$$

Applying duality shows that

$$2\zeta(3, 3, \mid a, b, c) - 2\zeta(3, (1,2) \mid b, c, a) + 2\zeta((1,2), (1,2) \mid c, a, b) \overset{1}{=} -2\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$$

So that we obtain a proof of (twice) Conjecture-Example 2.6.4 up to a rational, and in particular a proof of (twice) Hoffman's conjectural identity, up to a rational in the case $a = b = 0$.

Proof. To obtain the symmetrisation, Theorem 2.5.4 tell us to sum over all permutations of the block lengths. So we get the following $3! = 6$ terms

$$\begin{aligned}&I_{\mathrm{bl}}(2a+3, 2b+3, 2c+2) + I_{\mathrm{bl}}(2b+3, 2c+2, 2a+3) + I_{\mathrm{bl}}(2c+2, 2a+3, 2b+3) + \\ &+ I_{\mathrm{bl}}(2b+3, 2a+3, 2c+2) + I_{\mathrm{bl}}(2a+3, 2c+2, 2b+3) + I_{\mathrm{bl}}(2c+2, 2b+3, 2a+3)\,.\end{aligned}$$

Using Equations 2.6.2 to 2.6.4, we convert these back to the given MZV's up to ± 1. Since the weight is even, the result is in $\pi^{\mathrm{wt}}\mathbb{Q}$.

Moreover, each line is an instance of the cyclic insertion conjecture, so it expected to contribute one lot of $-\frac{\pi^{\text{wt}}}{(\text{wt}+1)!}$.

By duality, we have that $\zeta(3,3 \mid a,b,c) = \zeta((1,2),(1,2) \mid c,b,a)$, $\zeta(3,(1,2) \mid b,c,a) = \zeta(3,(1,2) \mid a,c,b)$, so the terms combine as indicated. ☐

Conjecture-Example 2.6.6 (Generalised Hoffman identity)**.** A higher version of Hoffman's identity arises from considering

$$z = (-1)^d \zeta(\{3\}^{2n} \mid a_1, \ldots, a_{2n}, c)\,,$$

where $d = 2n + \sum_i a_i + c$ is the depth. This has $2n+1$ blocks, and block decomposition

$$z = I_{\text{bl}}(2a_1+3, 2a_2+3, \ldots, 2a_{2n}+3, 2c+2)\,.$$

We calculate

$$\begin{aligned}
\mathcal{C}z &= (-1)^{d+1}\zeta(\{3\}^{2n-1}, (1,2) \mid a_2, \ldots, a_{2n}, c, a_1) \\
&= I_{\text{bl}}(2a_2+3, \ldots, 2a_{2n}+3, 2c+2, 2a_1+3) \\
\mathcal{C}^2 z &= (-1)^{d+2}\zeta(\{3\}^{2n-2}, \{(1,2)\}^2 \mid a_3, \ldots, a_{2n}, c, a_1, a_2) \\
&= I_{\text{bl}}(2a_3+3, \ldots, 2a_{2n}+3, 2c+2, 2a_1+3, 2a_2+3)\,.
\end{aligned}$$

And by induction

$$\mathcal{C}^i z = (-1)^d(-1)^i \zeta(\{3\}^{2n-i}, \{(1,2)\}^i \mid a_{i+1}, \ldots, a_{2n}, c, a_1, \ldots, a_i) \tag{2.6.5}$$

$$= I_{\text{bl}}(2a_{i+1}+3, \ldots, 2a_{2n}+3, 2c+2, 2a_1+3, \ldots, 2a_i+3)\,. \tag{2.6.6}$$

By Proposition 2.5.11 and Conjecture 2.5.1 we obtain

$$\begin{aligned}
\sum_{i=0}^{2n} \mathcal{C}^i z &= (-1)^d \sum_{i=0}^{2n} (-1)^i \zeta(\{3\}^{2n-i}, \{(1,2)\}^i \mid a_{i+1}, \ldots, a_{2n}, c, a_1, \ldots, a_i) \\
&\overset{?}{=} (-1)^{t/2} \frac{\pi^{t/2}}{(t+1)!}\,,
\end{aligned}$$

as the weight $t = 3 \times 2n + 2\sum_i a_i + 2c$ is even. Since $(-1)^{t/2} = (-1)^{n+d}$ we can write this as

$$\sum_{i=0}^{2n} (-1)^i \zeta(\{3\}^{2n-i}, \{(1,2)\}^i \mid a_{i+1}, \ldots, a_{2n}, c, a_1, \ldots, a_i) \overset{?}{=} (-1)^n \frac{\pi^{\text{wt}}}{(\text{wt}+1)!}\,.$$

Theorem 2.6.7 (Symmetrised generalised Hoffman identity)**.** *Symmetrising the generalised Hoffman identity, Conjecture-Example 2.6.6, using Theorem 2.5.4 shows the following identity holds,*

$$\begin{aligned}
&\sum_{\sigma \in S_{2n}} \sum_{i=0}^{2n} (-1)^i \zeta(\{3\}^{2n-i}, \{(1,2)\}^i \mid a_{\sigma(i+1)}, \ldots, a_{\sigma(2n)}, c, a_{\sigma(1)}, \ldots, a_{\sigma(i)}) \\
&\overset{1}{=} (-1)^n (2n)! \frac{\pi^{\text{wt}}}{(\text{wt}+1)!}\,.
\end{aligned}$$

Proof. Theorem 2.5.4 says we need to sum over all permutations of the block lengths. We can group these permutations by the position of the even length block $2c+2$ to obtain the following sum

$$\sum_{\sigma \in S_{2n}} \sum_{i=0}^{2n} I_{\mathrm{bl}}(2a_{\sigma(i+1)}+3, \ldots, 2a_{\sigma(2n)}+3, 2c+2, 2a_{\sigma(1)}+3, \ldots, 2a_{\sigma(i)}+3) \in \pi^{\mathrm{wt}}\mathbb{Q}\,.$$

Using Equation 2.6.6, this is converted into the MZV's above.

Moreover, for each fixed $\sigma \in S_{2n}$, we obtain a cyclic insertion conjecture identity of the original starting type as the inner sum. So this is a sum of $(2n)!$ cyclic insertion identities, each of which is expected to contribute $(-1)^n \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$. □

The above instances of the cyclic insertion conjecture have already been proposed. However, the generalised cyclic insertion conjecture Conjecture 2.5.1 can generate plenty of *new* identities which can be numerically verified. Henceforth we may begin to skip some details, since these ideas should now be familiar.

Notation 2.6.8. It is convenient to write $\zeta_{\mathcal{C}}(a_1, \ldots, a_n \mid b_1, \ldots, b_{n+1})$ to mean the sum obtained by applying the cyclic insertion conjecture to $\zeta(a_1, \ldots, a_n \mid b_1, \ldots, b_{n+1})$.

We will also use the notation $\mathrm{Sym}_{\{\, x_1, \ldots, x_n \,\}}$ to mean the sum of over all permutations of the variables x_i. That is

$$\mathrm{Sym}_{\{\, x_1, \ldots, x_n \,\}} f(x_1, \ldots, x_n) \coloneqq \sum_{\sigma \in S_n} f(x_{\sigma(1)}, \ldots, x_{\sigma(n)})$$

Conjecture-Example 2.6.9 ($\zeta(1,3,3,3)$)**.** Consider

$$z = (-1)^d \zeta(1,3,3,3 \mid a_1, a_2, a_3, a_4, a_5)\,,$$

where $d = 4 + \sum_i a_i$ is the depth. It has even weight $t = 10 + 2\sum_i a_i$, and block encoding

$$z = I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_4+3, 2a_5+2)\,,$$

with 5 blocks.

We find

$$\begin{aligned}
\mathcal{C}z &= (-1)^d \zeta(3,3,1,3 \mid a_3, a_4, a_5, a_1, a_2) = I_{\mathrm{bl}}(2a_3+3, 2a_4+3, 2a_5+2, 2a_1+2, 2a_2+2) \\
\mathcal{C}^2 z &= -(-1)^d \zeta(3,1,3,(1,2) \mid a_4, a_5, a_1, a_2, a_3) = I_{\mathrm{bl}}(2a_4+3, 2a_5+2, 2a_1+2, 2a_2+2, 2a_3+3) \\
\mathcal{C}^3 z &= (-1)^d \zeta(1,3,(1,2),(1,2) \mid a_5, a_1, a_2, a_3, a_4) = I_{\mathrm{bl}}(2a_5+2, 2a_1+2, 2a_2+2, 2a_3+3, 2a_4+3) \\
\mathcal{C}^4 z &= (-1)^d \zeta((1,2),(1,2),1,3 \mid a_2, a_3, a_4, a_5, a_1) = I_{\mathrm{bl}}(2a_2+2, 2a_3+3, 2a_4+3, 2a_5+2, 2a_1+2)\,.
\end{aligned}$$

Since $(-1)^{t/2} = (-1)^{1+d}$, we obtain the conjectural identity

$$\begin{aligned}
&\zeta_{\mathcal{C}}(1,3,3,3 \mid a_1, a_2, a_3, a_4, a_5) \\
&= \zeta(1,3,3,3 \mid a_1, a_2, a_3, a_4, a_5) + \zeta(3,3,1,3 \mid a_3, a_4, a_5, a_1, a_2) + \\
&\quad - \zeta(3,1,3,(1,2) \mid a_4, a_5, a_1, a_2, a_3) + \zeta(1,3,(1,2),(1,2) \mid a_5, a_1, a_2, a_3, a_4) + \\
&\quad + \zeta((1,2),(1,2),1,3 \mid a_2, a_3, a_4, a_5, a_1) \overset{?}{=} -\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.
\end{aligned}$$

Conjecture-Example 2.6.10 ($\zeta(1,3,3,(1,2))$)**.** Consider

$$z = (-1)^d \zeta(1,3,3,(1,2) \mid a_1,a_2,a_3,a_4,a_5)\,,$$

where $d = 5 + \sum_i a_i$ is the depth. It has even weight $t = 10 + 2\sum_i a_i$, and block encoding

$$z = I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_4+2, 2a_5+3)\,,$$

with 5 blocks.

We find

$$\begin{aligned}
\mathcal{C}z &= (-1)^d \zeta(3,(1,2),1,3 \mid a_3,a_4,a_5,a_1,a_2) = I_{\mathrm{bl}}(2a_3+3, 2a_4+2, 2a_5+3, 2a_1+2, 2a_2+2) \\
\mathcal{C}^2 z &= -(-1)^d \zeta((1,2),1,3,(1,2) \mid a_4,a_5,a_1,a_2,a_3) = I_{\mathrm{bl}}(2a_4+2, 2a_5+3, 2a_1+2, 2a_2+2, 2a_3+3) \\
\mathcal{C}^3 z &= (-1)^d \zeta((1,2),1,3,3 \mid a_2,a_3,a_4,a_5,a_1) = I_{\mathrm{bl}}(2a_2+2, 2a_3+3, 2a_4+2, 2a_5+3, 2a_1+2) \\
\mathcal{C}^4 z &= -(-1)^d \zeta(3,1,3,3 \mid a_5,a_1,a_2,a_3,a_4) = I_{\mathrm{bl}}(2a_5+3, 2a_1+2, 2a_2+2, 2a_3+3, 2a_4+2)\,.
\end{aligned}$$

Since $(-1)^{t/2} = (-1)^d$, we obtain the conjectural identity

$$\begin{aligned}
&\zeta_{\mathcal{C}}(1,3,3,(1,2) \mid a_1,a_2,a_3,a_4,a_5) \\
&= \zeta(1,3,3,(1,2) \mid a_1,a_2,a_3,a_4,a_5) + \zeta(3,(1,2),1,3 \mid a_3,a_4,a_5,a_1,a_2) + \\
&\quad - \zeta((1,2),1,3,(1,2) \mid a_4,a_5,a_1,a_2,a_3) + \zeta((1,2),1,3,3 \mid a_2,a_3,a_4,a_5,a_1) + \\
&\quad - \zeta(3,1,3,3 \mid a_5,a_1,a_2,a_3,a_4) \overset{?}{=} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.
\end{aligned}$$

Theorem 2.6.11. *Applying Theorem 2.5.4 to the identity in Conjecture-Example 2.6.9 above, shows the following identity holds*

$$\begin{aligned}
&\mathrm{Sym}_{\{1,2,5\}} \mathrm{Sym}_{\{3,4\}} \big(\zeta_{\mathcal{C}}(1,3,3,3 \mid a_1,a_2,a_3,a_4,a_5) \\
&\quad - \zeta_{\mathcal{C}}(1,3,3,(1,2) \mid a_1,a_2,a_3,a_5,a_4)\big) \overset{1}{=} -4!\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.
\end{aligned}$$

Notice this also works as a symmetrisation of Conjecture-Example 2.6.10.

Proof. If we symmetrise the above identity, we must sum over all permutations of block lengths. There are $5! = 120$ permutations. These are grouped into $5!/5 = 24$ cyclic insertion identities. The odd lengths can be permuted in $3! = 6$ ways without changing the type of MZV's which appear. Similarly the even lengths can be permuted in $2! = 2$ ways without changing the types of MZV's which appear. This reduces the number of permutations to consider to

$$\frac{5!}{5 \cdot 2! \cdot 3!} = 2\,.$$

These 'basic' permutations are

$$\begin{aligned}
&I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_4+3, 2a_5+2) \text{ and} \\
&I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_5+2, 2a_4+3)\,.
\end{aligned}$$

They do not differ by a cyclic shift because in the first the odd length block are consecutive, and in the second the odd length blocks are separated by 1. They respectively correspond to the MZV's

$$(-1)^d \zeta(1,3,3,3 \mid a_1, a_2, a_3, a_4, a_5) \text{ and}$$
$$- (-1)^d \zeta(1,3,3,(1,2) \mid a_1, a_2, a_3, a_5, a_4)\,,$$

where $d = 4 + \sum_i a_i$ is the depth of the *first* MZV.

To get all permutations from these, we sum over the cyclic shifts, giving the cyclic insertion terms above. We also sum over all permutations of a_1, a_2, a_5, and all permutations of a_3, a_4, giving the $\mathrm{Sym}_{\{1,2,5\}}$ and $\mathrm{Sym}_{\{3,4\}}$'s. Finally, each of the $24 = 4!$ cyclic insertion identities is expected to contribute $-\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$ to the total. □

Remark 2.6.12. In the case where the number of blocks n is *composite*, more care is necessary when choosing the representatives of all permutations modulo cyclic shifts, permutations of evens lengths and permutations of odd lengths. This is because $S_{\{\text{ even lengths }\}} \times S_{\{\text{ odd lengths }\}} \times C_n$ no longer acts freely on S_n.

For example in the case $n = 9$, the block decomposition

$$(2a_4 + 3, 2a_5 + 3, 2a_6 + 2, 2a_7 + 3, 2a_8 + 3, 2a_9 + 2, 2a_1 + 3, 2a_2 + 3, 2a_3 + 2)$$

is obtained from

$$(2a_1 + 3, 2a_2 + 3, 2a_3 + 2, 2a_4 + 3, 2a_5 + 3, 2a_6 + 2, 2a_7 + 3, 2a_8 + 3, 2a_9 + 2)$$

in two ways. It is obtained either by a cyclic shift of 3 left, or by permuting even lengths as (a_3, a_6, a_9) and the odd lengths as $(a_1, a_4, a_7)(a_2, a_5, a_8)$.

To work out the number of representatives, one could use Burnside's counting theorem. To work out the representatives, one can always first quotient by C_n and by the larger of $S_{\{\text{ even lengths }\}}$ or $S_{\{\text{ odd lengths }\}}$.

Conjecture-Example 2.6.13. Consider

$$z = \zeta(1,3,1,3,3,3 \mid a_1, a_2, a_3, a_4, a_5, a_6, a_7)\,,$$

where $d = 6 + \sum_i a_i$ is the depth. The weight $t = 14 + 2\sum_i a_i$ is even. And $(-1)^{t/2} = (-1)^{d+1} = -(-1)^d$. So applying the cyclic operator $\mathcal{C}$ gives the conjectural identity

$$\begin{aligned}
&\zeta_{\mathcal{C}}(1,3,1,3,3,3 \mid a_1, a_2, a_3, a_4, a_5, a_6, a_7) \\
&= \zeta(1,3,1,3,3,3 \mid a_1, a_2, a_3, a_4, a_5, a_6, a_7) + \\
&\quad + \zeta(1,3,3,3,1,3 \mid a_3, a_4, a_5, a_6, a_7, a_1, a_2) + \\
&\quad + \zeta(3,3,1,3,1,3 \mid a_5, a_6, a_7, a_1, a_2, a_3, a_4) + \\
&\quad - \zeta(3,1,3,1,3,(1,2) \mid a_6, a_7, a_1, a_2, a_3, a_4, a_5) +
\end{aligned}$$

$$\begin{aligned}
&+\zeta(1,3,1,3,(1,2),(1,2) \mid a_7,a_1,a_2,a_3,a_4,a_5,a_6)+\\
&+\zeta(1,3,(1,2),(1,2),1,3 \mid a_2,a_3,a_4,a_5,a_6,a_7,a_1)+\\
&+\zeta((1,2),(1,2),1,3,1,3 \mid a_4,a_5,a_6,a_7,a_1,a_2,a_3)\\
&\overset{?}{=} -\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.
\end{aligned}$$

Theorem 2.6.14. *The motivically proven symmetrisation of Conjecture-Example 2.6.13 is*

$$\begin{aligned}
&\mathrm{Sym}_{\{\,a_1,a_2,a_3,a_4,a_7\,\}}\,\mathrm{Sym}_{\{\,a_5,a_6\,\}}\Big(\zeta_{\mathcal{C}}(1,3,1,3,3,3 \mid a_1,a_2,a_3,a_4,a_5,a_6,a_7)+\\
&-\zeta_{\mathcal{C}}(1,3,(1,2),1,3,3 \mid a_1,a_2,a_3,a_5,a_4,a_6,a_7)+\\
&+\zeta_{\mathcal{C}}(1,3,3,1,3,3 \mid a_1,a_2,a_5,a_3,a_4,a_6,a_7)\Big)\\
&\overset{1}{=} -6!\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.
\end{aligned}$$

Proof. The integral corresponding to z has block decomposition

$$I_{\mathrm{bl}}(2a_1+2,2a_2+2,2a_3+2,2a_4+2,2a_5+3,2a_6+3,2a_7+2)\,,$$

with 7 block.

We must sum over all permutations of the lengths. Permuting the even block lengths $2a_1+2, 2a_2+2, 2a_3+2, 2a_4+2, 2a_7+2$ in 5! ways, and the odd block lengths $2a_5+3, 2a_6+3$ in 2! ways, will not change the type of MZV's which occur. This gives the $\mathrm{Sym}_{\{\,a_1,a_2,a_3,a_4,a_7\,\}}$ and $\mathrm{Sym}_{\{\,a_5,a_6\,\}}$. We can also group together the terms which come from the same cyclic insertion identity. This means grouping together 7 cyclic permutations of each block length.

This leaves $\frac{7!}{7\cdot 5!2!}=3$ permutations to consider. We find

$$\begin{aligned}
&I_{\mathrm{bl}}(2a_1+2,2a_2+2,2a_3+2,2a_4+2,2a_5+3,2a_6+3,2a_7+2)\\
&I_{\mathrm{bl}}(2a_1+2,2a_2+2,2a_3+2,2a_5+3,2a_4+2,2a_6+3,2a_7+2)\\
&I_{\mathrm{bl}}(2a_1+2,2a_2+2,2a_5+3,2a_3+2,2a_4+2,2a_6+3,2a_7+2)\,,
\end{aligned}$$

which give the MZV's above. □

Conjecture-Example 2.6.15. Consider

$$z=(-1)^d\zeta(1,3,3,3,3,3 \mid a_1,a_2,a_3,a_4,a_5,a_6,a_7)\,,$$

where $d=6+\sum_i a_i$ is the depth. The weight $t=16+2\sum_i a_i$ is even. And $(-1)^{t/2}=(-1)^{d+2}=(-1)^d$. So applying the cyclic operator $\mathcal{C}$ gives the conjectural identity

$$\begin{aligned}
&\zeta_{\mathcal{C}}(1,3,3,3,3,3 \mid a_1,a_2,a_3,a_4,a_5,a_6,a_7)\\
&=\zeta(1,3,3,3,3,3 \mid a_1,a_2,a_3,a_4,a_5,a_6,a_7)+\\
&\quad+\zeta(3,3,3,3,1,3, \mid a_3,a_4,a_5,a_6,a_7,a_1,a_2)+\\
&\quad-\zeta(3,3,3,1,3,(1,2) \mid a_4,a_5,a_6,a_7,a_1,a_2,a_3)+
\end{aligned}$$

$$\begin{aligned}
&+ \zeta(3,3,1,3,(1,2),(1,2) \mid a_5,a_6,a_7,a_1,a_2,a_3,a_4) + \\
&- \zeta(3,1,3,(1,2),(1,2),(1,2) \mid a_6,a_7,a_1,a_2,a_3,a_4,a_5) + \\
&+ \zeta(1,3,(1,2),(1,2),(1,2),(1,2) \mid a_7,a_1,a_2,a_3,a_4,a_5,a_6) + \\
&+ \zeta((1,2),(1,2),(1,2),(1,2),1,3 \mid a_2,a_3,a_4,a_5,a_6,a_7,a_1) \\
&\overset{?}{=} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!} \,.
\end{aligned}$$

Theorem 2.6.16. *The motivically proven symmetrisation of Conjecture-Example 2.6.15 is*

$$\begin{aligned}
&\mathrm{Sym}_{\{\, a_1,a_2,a_7 \,\}} \mathrm{Sym}_{\{\, a_3,a_4,a_5,a_6 \,\}} \Big(\zeta_{\mathcal{C}}(1,3,3,3,3,3 \mid a_1,a_2,a_3,a_4,a_5,a_6,a_7) + \\
&- \zeta_{\mathcal{C}}(1,3,3,3,3,(1,2) \mid a_1,a_2,a_3,a_4,a_5,a_7,a_6) + \\
&+ \zeta_{\mathcal{C}}(1,3,3,3,(1,2),(1,2) \mid a_1,a_2,a_3,a_4,a_7,a_5,a_6) + \\
&- \zeta_{\mathcal{C}}(1,3,3,(1,2),(1,2),(1,2) \mid a_1,a_2,a_3,a_7,a_4,a_5,a_6) + \\
&+ \zeta_{\mathcal{C}}((1,2),1,3,(1,2),(1,2),(1,2) \mid a_1,a_3,a_2,a_4,a_7,a_5,a_6) \Big) \\
&\overset{1}{=} 6! \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!} \,.
\end{aligned}$$

Proof. The integral corresponding to z has block decomposition

$$I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_4+3, 2a_5+3, 2a_6+3, 2a_7+2) \,,$$

with seven blocks.

We must sum over all permutations of the lengths. Permuting the even block lengths $2a_1+2, 2a_2+2, 2a_7+2$ in $3!$ ways, and the odd block lengths $2a_3+3, 2a_4+3, 2a_5+3, 2a_6+3$ in $4!$ ways, will not change the type of MZV's which occur. This gives the $\mathrm{Sym}_{\{\, a_1,a_2,a_7 \,\}}$ and $\mathrm{Sym}_{\{\, a_3,a_4,a_5,a_6 \,\}}$. We can also group together the terms which come from the same cyclic insertion identity. This means grouping together 7 cyclic permutations of each block length.

This leaves $\frac{7!}{7 \cdot 3! 4!} = 5$ permutations to consider. We find

$$\begin{aligned}
&I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_4+3, 2a_5+3, 2a_6+3, 2a_7+2) \\
&I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_4+3, 2a_5+3, 2a_7+2, 2a_6+3) \\
&I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_4+3, 2a_7+2, 2a_5+3, 2a_6+3) \\
&I_{\mathrm{bl}}(2a_1+2, 2a_2+2, 2a_3+3, 2a_7+2, 2a_4+3, 2a_5+3, 2a_6+3) \\
&I_{\mathrm{bl}}(2a_1+2, 2a_3+3, 2a_2+2, 2a_4+3, 2+2a_7, 2a_5+3, 2a_6+3) \,,
\end{aligned}$$

which give the MZV's above. □

It should be clear that we can continue stating conjectural identities, and producing provably true symmetrised versions which hold motivically, *ad nauseum*.

Before finishing this section, we will give two further examples of the cyclic insertion conjecture; one example in the odd weight case, and one example of what happens when it is applied in a 'degenerate' case.

Conjecture-Example 2.6.17. Consider

$$z = (-1)^d \zeta(1,3,3 \mid a_1, a_2, a_3, a_4)\,.$$

where $d = 3 + \sum_i a_i$. The weight $7 + 2\sum_i a_i$ is odd.

Applying the cyclic operator leads to the identity

$$\begin{aligned}\zeta_{\mathcal{C}}(1,3,3 \mid a_1,a_2,a_3,a_4) = {} & \zeta(1,3,3 \mid a_1,a_2,a_3,a_4) + \zeta(3,1,3 \mid a_3,a_4,a_1,a_2) + \\ & - \zeta(1,3,(1,2) \mid a_4,a_1,a_2,a_3) - \zeta((1,2),1,3 \mid a_2,a_3,a_4,a_1) \\ \overset{?}{=} {} & 0\,.\end{aligned}$$

(There is no point producing a symmetrisation in this case, since the terms will cancel pairwise using the duality of MZV's.)

Remark 2.6.18. It should be mentioned here that the above identity occurs when trying to investigate the exact BBBL cyclic insertion conjecture motivically. When computing $D_{<N}$, and attempting to check it vanishes, one obtains this combination of MZV's. In order for $D_{<N}$ to vanish this combination needs to be 0 motivically. A similar feature holds in other cases of the generalised cyclic insertion conjecture. See Example 2.6.19 a) for a specific example of this phenomenon.

This suggests that it might be possible to partially tackle the general conjecture motivically using some kind of recursion procedure. Indeed, Glanois [Gla16] has a notion of families of identities that are stable under the derivations. This allows her to lift analytically known families of identities to motivic identities, via recursion. The procedure, though, requires an analytic version of the identity to start the procedure, and to compute the rational at each step.

Other versions of cyclic insertion do always appear when computing the derivations D_{2k+1}. A subsequence which crosses i blocks, has α letters before it starts, and β letters after it finishes (as in Definition 2.2.29), gives rise to the following term in D_{2k+1}.

$$\begin{aligned}& I^{\mathfrak{m}}_{\text{bl}}(\ell_j, \ldots, \ell_n, \underbrace{\ell_1, \ell_2, \ldots, \ell_i}, \ell_{i+1}, \ldots, \ell_{j-1}) \\ & \quad \rightsquigarrow I^{\mathfrak{L}}_{\text{bl}}(\ell_1 - \alpha, \ell_2, \ldots, \ell_{i-1}, \ell_i - \beta) \otimes I^{\mathfrak{m}}_{\text{bl}}(\ell_j, \ldots, \ell_n, \ell_1 + \cdots + \ell_i - (2k+1), \ell_{i+1}, \ldots, \ell_{j-1})\,.\end{aligned}$$

By taking those cases where the blocks $\ell_1, \ldots, \ell_i$ are contiguous, we can mark the corresponding subsequence, as above. Thus in D_{2k+1} we obtain the $(n+1-i)$-term cyclic insertion identity

$$I^{\mathfrak{L}}_{\text{bl}}(\ell_1 - \alpha, \ell_2, \ldots, \ell_{i-1}, \ell_i - \beta) \otimes \sum_{\text{cycle}} I^{\mathfrak{m}}_{\text{bl}}(\ell_1 + \cdots + \ell_i - (2k+1), \ell_{i+1}, \ldots, \ell_n)\,.$$

The cases were $\ell_1, \ldots, \ell_i$ are not contiguous do not contribute anything to this, since the corresponding subsequence does not exist here.

One can potentially use this to make progress towards the conjecture. Knowledge of the cyclic insertion conjecture at all weights $< N$ could potentially be used to prove a motivic version of the cyclic insertion conjecture at weight N via cancellation in the derivations. However, a complete proof of the cyclic insertion conjecture at weight N would still require explicitly evaluating the rational factor, which cannot yet be done motivically. It is therefore unlikely that the conjecture can be resolved only using motivic MZV's,

Moreover, the computation and simplification of $D_{<N}$ in the odd weight cases appears to require *explicitly* eliminating products in the $I^{\mathfrak{L}}$ factor. See Example 2.6.19 b) for an example. In [Gla16], Glanois establishes new types of relations on the $I^{\mathfrak{L}}$ integrals, particularly the so-called ⧢-antipode relations, which could potentially be useful in this regard.

Example 2.6.19. a) For example, trying to prove $\zeta_{\mathcal{C}}(1,3,1,3 \mid 0,0,0,1,2) = \zeta_{\mathcal{C}}(1,3,1,2,3,2,2) \overset{1}{=} \frac{1}{15!}\pi^{14}$ motivicall y leads to the following computation.

$$\begin{aligned} D_3\zeta^{\mathfrak{m}}_{\mathcal{C}}(1,3,1,2,3,2,2) &= -3\zeta^{\mathfrak{L}}(3) \otimes \zeta^{\mathfrak{m}}_{\mathcal{C}}(1,2,2,3,3) + 3\zeta^{\mathfrak{L}}(3) \otimes \zeta^{\mathfrak{m}}_{\mathcal{C}}(1,2,3,2,3) \\ &= -3\zeta^{\mathfrak{L}}(3) \otimes \zeta^{\mathfrak{m}}_{\mathcal{C}}(1,3,3 \mid 0,2,0,0) + 3\zeta^{\mathfrak{L}}(3) \otimes \zeta^{\mathfrak{m}}_{\mathcal{C}}(1,3,3 \mid 0,1,1,0)\,. \end{aligned}$$

To conclude D_3 vanishes, we need to use (a motivic version of) Conjecture-Example 2.6.17, to say each summand is 0.

b) Moreover, trying to prove motivically that $\zeta_{\mathcal{C}}(1,3,3 \mid 0,2,0,0) = \zeta_{\mathcal{C}}(1,2,2,3,3) = 0$ leads to the following computation (after replacing $\zeta^{\mathfrak{m}}(1,3) = \frac{1}{3}\zeta^{\mathfrak{m}}(2,2)$).

$$\begin{aligned} D_7\zeta_{\mathcal{C}}(1,3,3 \mid 0,2,0,0) = (&-5\zeta^{\mathfrak{L}}(1,3,3) - \zeta^{\mathfrak{L}}(2,2,3) - \zeta^{\mathfrak{L}}(2,3,2) - 2\zeta^{\mathfrak{L}}(3,1,3) + \\ &- 2\zeta^{\mathfrak{L}}(3,2,2) - 3\zeta^{\mathfrak{L}}(2,1,1,3)) \otimes \zeta^{\mathfrak{m}}(2,2)\,. \end{aligned}$$

To conclude D_7 vanishes, we need to recognise the $\mathfrak{L}$ factor can be written

$$= -\zeta^{\mathfrak{L}}(2)\zeta^{\mathfrak{L}}(2,3) - 2\zeta^{\mathfrak{L}}(2)\zeta^{\mathfrak{L}}(3,2) + 2\zeta^{\mathfrak{L}}(3)\zeta^{\mathfrak{L}}(2,2)\,.$$

This does now vanish because in the $\mathfrak{L}$ factor we work modulo products.

Finally, here is an example of cyclic insertion in a 'degenerate' case.

Conjecture-Example 2.6.20. Consider

$$z = (-1)^d\zeta(3,(1,2),\{2\}^a,(1,2),1,3,\{2\}^a,3,3,(1,2),\{2\}^a)\,,$$

where $d = 11 + 3a$ is the depth. The weight $t = 22 + 6a$ is even. Notice we have $(-1)^d = (-1)^{t/2}$.

If we apply $\mathcal{C}$ in this case we obtain

$$\begin{aligned} \mathcal{C}z &= -(-1)^d\zeta((1,2),\{2\}^a,(1,2),1,3,\{2\}^a,3,3,(1,2),\{2\}^a,(1,2)) \\ \mathcal{C}^2z &= -(-1)^d\zeta(\{2\}^a,3,3,(1,2),\{2\}^a,(1,2),1,3,\{2\}^a,3,3)\,. \end{aligned}$$

Then, surprisingly, we have $\mathcal{C}^3 z = z$. So we have $\sum_{i=0}^{8} \mathcal{C}^i z = 3 \sum_{i=0}^{2} \mathcal{C}^i$, and by dividing through we obtain the following conjectural identity

$$\begin{aligned}
&\zeta(3,(1,2),\{2\}^a,(1,2),1,3,\{2\}^a,3,3,(1,2),\{2\}^a) + \\
&-\zeta((1,2),\{2\}^a,(1,2),1,3,\{2\}^a,3,3,(1,2),\{2\}^a,(1,2)) + \\
&-\zeta(\{2\}^a,3,3,(1,2),\{2\}^a,(1,2),1,3,\{2\}^a,3,3) \\
&\overset{?}{=} \frac{3}{9}\frac{\pi^{\text{wt}}}{(\text{wt}+1)!}\,.
\end{aligned}$$

One can check numerically this appears to be the case, to at least 5000 decimal places, for various small values of a.

2.7 Other motivically provable symmetrisations

The above framework shows that all cyclic insertion identities can be sufficienly symmetrised in order to obtain a motivically provable identity. The symmetrisation procedure above happens in a very particular way. This means that there are plenty of motivically provable identities which do hold, but fall outside the scope of this framework. In this section we will present some identities that can be motivically proven, but not using Theorem 2.5.4.

2.7.1 $\zeta_{\mathcal{C}}(1,3,3,(1,2) \mid 0,0,0,0,n)$

Theorem 2.7.1. *The following identity, a cyclic insertion identity on the nose, can be motivically proven.*

$$\begin{aligned}
&\zeta_{\mathcal{C}}(1,3,3,(1,2) \mid 0,0,0,0,n) \\
&= \zeta(1,3,3,(1,2) \mid 0,0,0,0,n) + \zeta(3,(1,2),1,3, \mid 0,0,n,0,0) + \\
&\quad -\zeta((1,2),1,3,(1,2) \mid 0,n,0,0,0) + \zeta((1,2),1,3,3 \mid 0,0,0,n,0) + \\
&\quad -\zeta(3,1,3,3 \mid n,0,0,0,0) \overset{1}{=} \frac{\pi^{\text{wt}}}{(\text{wt}+1)!}
\end{aligned}$$

The identity would, a priori, fall into the symmetrisation given in Theorem 2.6.11, and include 6 times as many terms. But, by good fortune, this is not necessary.

Proof. This is a cyclic insertion conjecture identity. The generating MZV has depth $d = 5+n$, and the weight $t = 10+2n$. Since $(-1)^d = (-1)^{t/2}$, we expect the value to be $+\frac{\pi^{\text{wt}}}{(\text{wt}+1)!}$.

To really begin the proof, let's first write down the terms generated in this identity in their full form. We find

$$\begin{aligned}
&\zeta(\{2\}^n,1,3,3,1,2) + \zeta(3,1,2,1,\{2\}^n,3) - \zeta(1,2,1,\{2\}^n,3,1,2) + \\
&+\zeta(1,2,1,3,3,\{2\}^n) - \zeta(3,\{2\}^n,1,3,3) \overset{1}{=} \frac{\pi^{2n+10}}{(2n+11)!}
\end{aligned}$$

Now we compute $D_{2\ell+1}$ on each term of this identity.

First term

The first term of this identity corresponds to the integral

$$I^{\mathfrak{m}}(0(10)^n 1 \mid 10 \mid 010 \mid 01 \mid 101) = I^{\mathfrak{m}}((01)^{n+1} \parallel 10 \mid 010 \mid 01 \mid 101)\,.$$

We distinguish subsequences (hence terms of D_k) by their location on the integral – either in the *Left* half before $\|$, in the *Right* half after it, or covering both halves. Since $k = 2\ell + 1$ is necessarily odd, we will track the operator a term contributes to by ℓ.

L: Any subsequence lying in the left half is automatically trivial because it starts and ends with the same symbol (remember k is odd).

R: We can systematically list the terms by labelling the positions in the string

$$I^{\mathfrak{m}}((01)^{n+1} \parallel \overset{1}{1}\overset{2}{0}\overset{3}{0}\overset{4}{1}\overset{5}{0}\overset{6}{0}\overset{7}{1}\overset{8}{1}\overset{9}{0}\overset{10}{1})\,,$$

and looking for labels of the same parity which contain different letters. We find

$$\begin{aligned}
&\text{1–5:} && I^{\mathfrak{L}}(10010) \otimes I^{\mathfrak{m}}((01)^{n+1}1 \mid 001101) && \text{for } \ell = 1 && \text{(1Ra)}\\
&\text{1–9:} && I^{\mathfrak{L}}(100100110) \otimes I^{\mathfrak{m}}((01)^{n+1}1 \mid 01) && \text{for } \ell = 3 && \text{(1Rb)}\\
&\text{2–8:} && I^{\mathfrak{L}}(0010011) \otimes I^{\mathfrak{m}}((01)^{n+1}10 \mid 101) && \text{for } \ell = 2 && \text{(1Rc)}\\
&\text{2–10:} && I^{\mathfrak{L}}(001001101) \otimes I^{\mathfrak{m}}((01)^{n+1}10 \mid 1) && \text{for } \ell = 3 && \text{(1Rd)}\\
&\text{3–7:} && I^{\mathfrak{L}}(01001) \otimes I^{\mathfrak{m}}((01)^{n+1}100 \mid 1101) && \text{for } \ell = 1 && \text{(1Re)}\\
&\text{6–10:} && I^{\mathfrak{L}}(01101) \otimes I^{\mathfrak{m}}((01)^{n+1}100100 \mid 1) && \text{for } \ell = 1 && \text{(1Rf)}
\end{aligned}$$

Notice that term (1Ra) cancels with (1Re).

LR: By replicating the 01 pattern from the left hand side through into the right, we see that the only terms which can contribute are those with odd label and letter 1, or those with even label and letter 0. We find for $k = 2\ell + 1$, the following possibilities

$$\begin{aligned}
&\text{end at 1:} && I^{\mathfrak{L}}(01(01)^{\ell}1) \otimes I^{\mathfrak{m}}((01)^{n-\ell}0 \mid 1001001101) && \text{for } 1 \leq \ell \leq n && \text{(1LRa)}\\
&\text{end at 2:} && I^{\mathfrak{L}}(1(01)^{\ell}10) \otimes I^{\mathfrak{m}}((01)^{n-\ell}01 \mid 001001101) && \text{for } 1 \leq \ell \leq n && \text{(1LRb)}\\
&\text{end at 6:} && I^{\mathfrak{L}}(1(01)^{\ell-2}100100) \otimes I^{\mathfrak{m}}((01)^{n-\ell-2}01 \mid 01101) && \text{for } 2 \leq \ell \leq n+2 && \text{(1LRc)}\\
&\text{end at 7:} && I^{\mathfrak{L}}(01(01)^{\ell-3}1001001) \otimes I^{\mathfrak{m}}((01)^{n-\ell-3}0 \mid 1101) && \text{for } 3 \leq \ell \leq n+3 && \text{(1LRd)}
\end{aligned}$$

Second Term

The integral is $I^{\mathfrak{m}}(01001101 \parallel (10)^{n+1} \parallel 01)$. This time we have terms in the *Middle* of the two $\|$'s. We get terms

L:
$$I^{\mathfrak{L}}(01001) \otimes I^{\mathfrak{m}}(01 \mid 101(10)^{n+1}01) \quad \text{for } \ell = 1 \tag{2La}$$
$$I^{\mathfrak{L}}(01101) \otimes I^{\mathfrak{m}}(0100 \mid 1(10)^{n+1}01) \quad \text{for } \ell = 1 \tag{2Lb}$$

M and R: None.

LM:
$$I^{\mathfrak{L}}(01001101(10)^{\ell-3}1) \otimes I^{\mathfrak{m}}(0 \mid 10(10)^{n-\ell+3}01) \quad \text{for } 3 \leq \ell \leq n+3 \tag{2LMa}$$
$$I^{\mathfrak{L}}(1001101(10)^{\ell-3}10) \otimes I^{\mathfrak{m}}(01 \mid 0(10)^{n-\ell+3}01) \quad \text{for } 3 \leq \ell \leq n+3 \tag{2LMb}$$
$$I^{\mathfrak{L}}(001101(10)^{\ell-2}1) \otimes I^{\mathfrak{m}}(010 \mid 10(10)^{n-\ell+2}01) \quad \text{for } 2 \leq \ell \leq n+2 \tag{2LMc}$$
$$I^{\mathfrak{L}}(101(10)^{\ell-1}10) \otimes I^{\mathfrak{m}}(010011 \mid 0(10)^{n-\ell+1}01) \quad \text{for } 1 \leq \ell \leq n+1 \tag{2LMd}$$
$$I^{\mathfrak{L}}(01(10)^{\ell}1) \otimes I^{\mathfrak{m}}(0100110 \mid 10(10)^{n-\ell}01) \quad \text{for } 1 \leq \ell \leq n \tag{2LMe}$$
$$I^{\mathfrak{L}}(1(10)^{\ell}10) \otimes I^{\mathfrak{m}}(01001101 \mid 0(10)^{n-\ell}01) \quad \text{for } 1 \leq \ell \leq n \tag{2LMf}$$

MR:
$$I^{\mathfrak{L}}(10(10)^{\ell}0) \otimes I^{\mathfrak{m}}(01001101(10)^{n-\ell}1 \mid 01) \quad \text{for } 1 \leq \ell \leq n \tag{2MRa}$$
$$I^{\mathfrak{L}}(0(10)^{\ell}01) \otimes I^{\mathfrak{m}}(01001101(10)^{n-\ell}10 \mid 1) \quad \text{for } 1 \leq \ell \leq n \tag{2MRb}$$

LMR:
$$I^{\mathfrak{L}}(01101(10)^{n+1}01) \otimes I^{\mathfrak{m}}(0100 \mid 1) \quad \text{for } \ell = n+3 \tag{2LMRa}$$
$$I^{\mathfrak{L}}(1101(10)^{n+1}0) \otimes I^{\mathfrak{m}}(01001 \mid 01) \quad \text{for } \ell = n+2 \tag{2LMRb}$$

Third Term

The integral is $I^{\mathfrak{m}}(01101 \parallel (10)^{n+1} \parallel 01101)$

L:
$$I^{\mathfrak{L}}(01101) \otimes I^{\mathfrak{m}}(0 \mid 1(10)^{n+1}01101) \quad \text{for } \ell = 1 \tag{3La}$$

M: None.

R:
$$I^{\mathfrak{L}}(01101) \otimes I^{\mathfrak{m}}(01101(10)^{n+1}0 \mid 1) \quad \text{for } \ell = 1 \tag{3Ra}$$

LM:
$$I^{\mathfrak{L}}(101(10)^{\ell-1}10) \otimes I^{\mathfrak{m}}(011 \mid 0(10)^{n-\ell+1}01101) \quad \text{for } 1 \leq \ell \leq n+1 \tag{3LMa}$$
$$I^{\mathfrak{L}}(01(10)^{\ell}1) \otimes I^{\mathfrak{m}}(0110 \mid 10(10)^{n-\ell}01101) \quad \text{for } 1 \leq \ell \leq n \tag{3LMb}$$
$$I^{\mathfrak{L}}(1(10)^{\ell}10) \otimes I^{\mathfrak{m}}(01101 \mid 0(10)^{n-\ell}01101) \quad \text{for } 1 \leq \ell \leq n \tag{3LMc}$$

MR:
$$I^{\mathfrak{L}}(10(10)^{\ell}0) \otimes I^{\mathfrak{m}}(01101(10)^{n-\ell}1 \mid 01101) \quad \text{for } 1 \leq \ell \leq n \tag{3MRa}$$
$$I^{\mathfrak{L}}(0(10)^{\ell}01) \otimes I^{\mathfrak{m}}(01101(10)^{n-\ell}10 \mid 1101) \quad \text{for } 1 \leq \ell \leq n \tag{3MRb}$$

LMR:
$$I^{\mathfrak{L}}(01101(10)^{n+1}01) \otimes I^{\mathfrak{m}}(0 \mid 1101) \quad \text{for } \ell = n+3 \tag{3LMRa}$$
$$I^{\mathfrak{L}}(1101(10)^{n+1}0) \otimes I^{\mathfrak{m}}(01 \mid 01101) \quad \text{for } \ell = n+2 \tag{3LMRb}$$
$$I^{\mathfrak{L}}(101(10)^{n+1}0110) \otimes I^{\mathfrak{m}}(011 \mid 01) \quad \text{for } \ell = n+3 \tag{3LMRc}$$
$$I^{\mathfrak{L}}(01(10)^{n+1}011) \otimes I^{\mathfrak{m}}(0110 \mid 101) \quad \text{for } \ell = n+2 \tag{3LMRd}$$

$$I^{\mathfrak{L}}(01(10)^{n+1}01101) \otimes I^{\mathfrak{m}}(0110 \mid 1) \quad \text{for } \ell = n+3 \tag{3LMRe}$$

$$I^{\mathfrak{L}}(1(10)^{n+1}0110) \otimes I^{\mathfrak{m}}(01101 \mid 01) \quad \text{for } \ell = n+2 \tag{3LMRf}$$

Fourth term

The integral is $I^{\mathfrak{m}}(0110110010 \parallel (01)^{n+1})$.

L:

$$I^{\mathfrak{L}}(01101) \otimes I^{\mathfrak{m}}(0 \mid 110010(01)^{n+1}) \quad \text{for } \ell = 1 \tag{4La}$$

$$I^{\mathfrak{L}}(011011001) \otimes I^{\mathfrak{m}}(0 \mid 10(01)^{n+1}) \quad \text{for } \ell = 3 \tag{4Lb}$$

$$I^{\mathfrak{L}}(1101100) \otimes I^{\mathfrak{m}}(01 \mid 010(01)^{n+1}) \quad \text{for } \ell = 2 \tag{4Lc}$$

$$I^{\mathfrak{L}}(110110010) \otimes I^{\mathfrak{m}}(01 \mid 0(01)^{n+1}) \quad \text{for } \ell = 3 \tag{4Ld}$$

$$I^{\mathfrak{L}}(10110) \otimes I^{\mathfrak{m}}(011 \mid 0010(01)^{n+1}) \quad \text{for } \ell = 1 \tag{4Le}$$

$$I^{\mathfrak{L}}(10010) \otimes I^{\mathfrak{m}}(011011 \mid 0(01)^{n+1}) \quad \text{for } \ell = 1 \tag{4Lf}$$

Notice that term (4La) cancels with (4Le).

LR:

$$I^{\mathfrak{L}}(10110010(01)^{\ell-3}0) \otimes I^{\mathfrak{m}}(011 \mid 01(01)^{n-\ell+3}) \quad \text{for } 3 \le \ell \le n+3 \tag{4LRa}$$

$$I^{\mathfrak{L}}(0110010(01)^{\ell-3}01) \otimes I^{\mathfrak{m}}(0110 \mid 1(01)^{n-\ell+3}) \quad \text{for } 3 \le \ell \le n+3 \tag{4LRb}$$

$$I^{\mathfrak{L}}(110010(01)^{\ell-2}0) \otimes I^{\mathfrak{m}}(01101 \mid 01(01)^{n-\ell+2}) \quad \text{for } 2 \le \ell \le n+2 \tag{4LRc}$$

$$I^{\mathfrak{L}}(010(01)^{\ell-1}01) \otimes I^{\mathfrak{m}}(01101100 \mid 1(01)^{n-\ell+1}) \quad \text{for } 1 \le \ell \le n+1 \tag{4LRd}$$

$$I^{\mathfrak{L}}(10(01)^{\ell}0) \otimes I^{\mathfrak{m}}(011011001 \mid 01(01)^{n-\ell}) \quad \text{for } 1 \le \ell \le n \tag{4LRe}$$

$$I^{\mathfrak{L}}(0(01)^{\ell}01) \otimes I^{\mathfrak{m}}(0110110010 \mid 1(01)^{n-\ell}) \quad \text{for } 1 \le \ell \le n \tag{4LRf}$$

Fifth term

The integral is $I^{\mathfrak{m}}(010 \parallel (01)^{n+1} \parallel 1001001))$.

R:

$$I^{\mathfrak{L}}(10010) \otimes I^{\mathfrak{m}}(010(01)^{n+1}1 \mid 001) \quad \text{for } \ell = 1 \tag{5Ra}$$

$$I^{\mathfrak{L}}(01001) \otimes I^{\mathfrak{m}}(010(01)^{n+1}100 \mid 1) \quad \text{for } \ell = 1 \tag{5Rb}$$

LM:

$$I^{\mathfrak{L}}(010(01)^{\ell-1}01) \otimes I^{\mathfrak{m}}(0 \mid 1(01)^{n+1-\ell}1001001) \quad \text{for } 1 \le \ell \le n+1 \tag{5LMa}$$

$$I^{\mathfrak{L}}(10(01)^{\ell}0) \otimes I^{\mathfrak{m}}(01 \mid 01(01)^{n-\ell}1001001) \quad \text{for } 1 \le \ell \le n \tag{5LMb}$$

$$I^{\mathfrak{L}}(0(01)^{\ell}01) \otimes I^{\mathfrak{m}}(010 \mid 1(01)^{n-\ell}1001001) \quad \text{for } 1 \le \ell \le n \tag{5LMc}$$

MR:

$$I^{\mathfrak{L}}(01(01)^{\ell}1) \otimes I^{\mathfrak{m}}(010(01)^{n-\ell}0 \mid 1001001) \quad \text{for } 1 \le \ell \le n \tag{5MRa}$$

$$I^{\mathfrak{L}}(1(01)^{\ell}10) \otimes I^{\mathfrak{m}}(010(01)^{n-\ell}01 \mid 001001) \quad \text{for } 1 \le \ell \le n \tag{5MRb}$$

$$I^{\mathfrak{L}}(1(01)^{\ell-2}100100) \otimes I^{\mathfrak{m}}(010(01)^{n-\ell+2}01 \mid 01) \quad \text{for } 2 \le \ell \le n+2 \tag{5MRc}$$

$$I^{\mathfrak{L}}(01(01)^{\ell-3}1001001) \otimes I^{\mathfrak{m}}(010(01)^{n-\ell+3}0 \mid 1) \quad \text{for } 3 \le \ell \le n+3 \tag{5MRd}$$

LMR:

$$I^{\mathfrak{L}}(010(01)^{n+1}1001) \otimes I^{\mathfrak{m}}(0 \mid 1001) \quad \text{for } \ell = n+3 \tag{5LMRa}$$

$$I^{\mathfrak{L}}(10(01)^{n+1}100) \otimes I^{\mathfrak{m}}(01 \mid 01001) \quad \text{for } \ell = n+2 \tag{5LMRb}$$

$$I^{\mathfrak{L}}(10(01)^{n+1}10010) \otimes I^{\mathfrak{m}}(01 \mid 001) \quad \text{for } \ell = n+3 \tag{5LMRc}$$

$$I^{\mathfrak{L}}(0(01)^{n+1}1001) \otimes I^{\mathfrak{m}}(010 \mid 1001) \quad \text{for } \ell = n+2 \tag{5LMRd}$$

Now we attempt to see which terms cancel, and how they do so. The following series of lemmas identify the cancellation between all terms in $D_{<N}$.

Lemma 2.7.2. *The remaining terms from* (1Ra)–(1Rf) *cancel with those from* (4La)–(4Lf)*, as follows*

$$\begin{aligned} I^{\mathfrak{m}}((01)^{n+1} \parallel \underbracket{10 \mid 010 \mid 01 \mid 101}) &\leftrightarrow I^{\mathfrak{m}}((01)^{n+1} \parallel \underbracket{101 \mid 10 \mid 010 \mid 01}) \\ &= I^{\mathfrak{m}}(\underbracket{01 \mid 101 \mid 10 \mid 010} \parallel (01)^{n+1}) \end{aligned}$$

Lemma 2.7.3. *The terms from* (1LRa)–(1LRb) *cancel with the terms from* (2MRa)–(2MRb)*, as follows*

$$\begin{aligned} I^{\mathfrak{m}}(\underbracket{(01)^{n+1} \parallel 10} \mid 010 \mid 01 \mid 101) &\leftrightarrow I^{\mathfrak{m}}(\underbracket{01 \parallel (10)^{n+1}} \parallel 010 \mid 01 \mid 101) \\ &= I^{\mathfrak{m}}(010 \mid 01 \mid 101 \parallel \underbracket{(10)^{n+1} \parallel 01}) \,. \end{aligned}$$

Lemma 2.7.4. *The terms* (1LRc)–(1LRd) *cancels with the terms* (5MRc)–(5MRd)*, as follows*

$$\begin{aligned} I^{\mathfrak{m}}(\underbracket{(01)^{n+1} \parallel 10 \mid 010 \mid 01} \mid 101) &\leftrightarrow I^{\mathfrak{m}}(\underbracket{01 \mid 101 \mid 10 \parallel (01)^{n+1}} \parallel 101) \\ &= I^{\mathfrak{m}}(010 \parallel \underbracket{(01)^{n+1} \parallel 10 \mid 010 \mid 01}) \end{aligned}$$

Lemma 2.7.5. *The terms* (2La) *cancel with* (3Ra)*, and* (2Lb) *cancel with* (3La) *via*

$$I^{\mathfrak{m}}(\underbracket{010 \mid 01} \mid 101 \parallel (10)^{n+1} \parallel 01) \leftrightarrow I^{\mathfrak{m}}(01 \mid 101 \parallel (10)^{n+1} \parallel \underbracket{01 \mid 101}) \,,$$

and

$$I^{\mathfrak{m}}(010 \mid \underbracket{01 \mid 101} \parallel (10)^{n+1} \parallel 01) \leftrightarrow I^{\mathfrak{m}}(\underbracket{01 \mid 101} \parallel (10)^{n+1} \parallel 01 \mid 101) \,.$$

Lemma 2.7.6. *The terms* (2LMa)–(2LMc) *cancel with* (4LRa)–(4LRc) *via*

$$\begin{aligned} I^{\mathfrak{m}}(\underbracket{\boxed{010} \mid 01 \mid 101 \parallel (10)^{n+1}} \parallel 01) &\leftrightarrow I^{\mathfrak{m}}(\underbracket{(01)^{n+1} \parallel 101 \mid 10 \mid \boxed{010}} \mid 01) \\ &= I^{\mathfrak{m}}(01 \mid \underbracket{\boxed{101} \mid 10 \mid 010 \parallel (01)^{n+1}}) \,. \end{aligned}$$

Lemma 2.7.7. *The terms* (2LMd)–(2LMf) *cancel with* (3LMa)–(3LMc) *via*

$$\begin{aligned} I^{\mathfrak{m}}(010 \mid 01 \mid \underbracket{101 \parallel (10)^{n+1}} \parallel 01) &\leftrightarrow I^{\mathfrak{m}}(010 \mid 01 \parallel \underbracket{(10)^{n+1} \parallel 010} \mid 01) \\ &= I^{\mathfrak{m}}(01 \mid \underbracket{101 \parallel (10)^{n+1}} \parallel 01 \mid 101) \,. \end{aligned}$$

Lemma 2.7.8. *The terms* (4LRd)–(4LRf) *cancel with* (5LMa)–(5LMc) *via*

$$I^{\mathfrak{m}}(01 \mid 101 \mid 10 \mid \underbracket{\boxed{010} \parallel (01)^{n+1}} \leftrightarrow I^{\mathfrak{m}}(01 \mid 101 \mid 10 \parallel \underbracket{(01)^{n+1} \parallel \boxed{101}})$$

$$= I^{\mathfrak{m}}(\underbracket{\boxed{010} \parallel (01)^{n+1}} \parallel 10 \mid 010 \mid 01)\,.$$

Lemma 2.7.9. *The terms* (3MRa)–(3MRb) *cancel with* (5MRa)–(5MRb) *via*

$$\begin{aligned} I^{\mathfrak{m}}(01 \mid 101 \parallel \underbracket{(10)^{n+1} \parallel 01} \mid 101) &\leftrightarrow I^{\mathfrak{m}}(01 \mid 101 \mid \underbracket{10 \parallel (01)^{n+1}} \parallel 101) \\ &= I^{\mathfrak{m}}(010 \parallel \underbracket{(01)^{n+1} \parallel 10} \mid 010 \mid 01)\,. \end{aligned}$$

Lemma 2.7.10. *The terms* (2LMRa)–(2LMRb) *cancel with* (3LMRa)–(3LMRb) *via*

$$\begin{aligned} I^{\mathfrak{m}}(010 \mid \underbracket{01 \mid 101 \parallel (10)^{n+1} \parallel 01}) &\leftrightarrow I^{\mathfrak{m}}(010 \mid \underbracket{01 \parallel (10)^{n+1} \parallel 010 \mid 01}) \\ &= I^{\mathfrak{m}}(\underbracket{01 \mid 101 \parallel (10)^{n+1} \parallel 01} \mid 101)\,. \end{aligned}$$

Lemma 2.7.11. *The terms* (3LMRc)–(3LMRf) *cancel with* (5LMRa)–(5LMRb) *via*

$$\begin{aligned} I^{\mathfrak{m}}(01 \mid \underbracket{101 \parallel (10)^{n+1} \parallel 01 \mid 101}) &\leftrightarrow I^{\mathfrak{m}}(01 \mid \underbracket{101 \mid 10 \parallel (01)^{n+1} \parallel 101}) \\ &= I^{\mathfrak{m}}(\underbracket{010 \parallel (01)^{n+1} \parallel 10 \mid 010} \mid 01)\,. \end{aligned}$$

These lemmas show that all the terms in $D_{<N}$ cancel. So using Brown's characterisation of $\ker D_{<N}$ in Theorem 1.2.15, we conclude that this combination is a rational multiple of π^{wt}, as claimed. ☐

Remark 2.7.12. Alongside the usual reflection of blocks, this cancellation could be seen to involve a kind of 'splice' operation where a substring is cut out from one place, and stitched into a different place. This occurs in Lemma 2.7.5. It also involves a kind of 'extended reflection'. For example in cancelling (1Ra) with (1Re), the subsequence lies over blocks 2 and 3, but the cancellation occurs by reflecting blocks 2, 3 and 4.

2.7.2 $\sum_{\textbf{weak compositions}} \zeta_{\mathcal{C}}(1,3,3,3, \mid a_1, \ldots, a_5)$

We can give a different symmetrisation of the $\zeta_{\mathcal{C}}(1,3,3,3 \mid a_1, \ldots, a_5)$ identity from Theorem 2.6.11. This symmetrisation is very reminiscent of the Bowman-Bradley theorem from [BB02] (Theorem 2.1.7 above), involving a sum over all weak compositions. (Recall, weak compositions are compositions $\sum_i a_i = m$, where parts $a_i = 0$ are allowed).

Theorem 2.7.13. *The following identity is motivically provable*

$$\sum_{\substack{a_1 + \cdots + a_5 = m \\ a_i \geq 0}} \zeta_{\mathcal{C}}(1,3,3,3 \mid a_1, \ldots, a_5) \overset{1}{=} -\binom{5+m}{m} \frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\,.$$

Proof sketch. Firstly, it is a standard result that there are $\binom{5+m}{m}$ weak compositions of m into 5 parts. Since the generating MZV has depth $4 + \sum a_i$, and weight $t = 10 + 2\sum_i a_i$, we have $(-1)^d = -(-1)^{t/2}$, we expect each cyclic insertion identity to contribute $-\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}$.

Now we need to show all the terms in $D_{<N}$ cancel. We will only sketch the ideas for this proof, without making all of the details precise.

We have five types of terms with the corresponding integrals (up to $\pm$)

$$\zeta(1,3,3,3 \mid a,b,c,d,e) = I((01)^{a+1}(10)^{b+1}(01)^{c+1}\boxed{00}(10)^{d+1}(01)^{e+1}) \tag{Type 1}$$

$$\zeta(3,3,1,3 \mid a,b,c,d,e) = I((01)^{a+1}\boxed{00}(10)^{b+1}(01)^{c+1}(10)^{d+1}(01)^{e+1}) \tag{Type 2}$$

$$-\zeta(3,1,3,(1,2) \mid a,b,c,d,e) = I(\boxed{0}(10)^{a+1}(01)^{b+1}(10)^{c+1}(01)^{d+1}(10)^{e+1}\boxed{1}) \tag{Type 3}$$

$$\zeta(1,3,(1,2),(1,2) \mid a,b,c,d,e) = I((01)^{a+1}(10)^{b+1}(01)^{c+1}(10)^{d+1}\boxed{11}(01)^{e+1}) \tag{Type 4}$$

$$\zeta((1,2),(1,2),1,3 \mid a,b,c,d,e) = I((01)^{a+1}(10)^{b+1}\boxed{11}(01)^{c+1}(10)^{d+1}(01)^{e+1})\,. \tag{Type 5}$$

Any subsequence which does not intersect $\boxed{00}$, and does not intersect $\boxed{11}$, can be made to cancel by reflecting the blocks which contain the subsequence. For (Type 1), this entails

$$I(\overbrace{(\underbracket{0\,1)^{a+1}(10}_{})^{b+1}}^{\text{reflect}}(01)^{c+1}\boxed{00}(10)^{d+1}(01)^{e+1}) \leftrightarrow I((\underbracket{01)^{b+1}(1}_{}\,0)^{a+1}(01)^{c+1}\boxed{00}(10)^{d+1}(01)^{e+1})\,.$$

Notice that the cancellation happens within an integral of the same type, with some permutation of the lengths a_i. The sum over all weak compositions includes all permutations of the individual a_i, so this cancellation is okay.

In integrals of (Type 1), (Type 2), (Type 4) or (Type 5), any subsequence which crosses $\boxed{00}$ or $\boxed{11}$ and ends away from it can be made to cancel by reflecting the containing blocks. In this case, some integrals of (Type 1) cancel with integrals of (Type 2), with some permutation of the a_i, as follows

$$I(\overbrace{(\underbracket{0\,1)^{a+1}(10)^{b+1}(01)^{c+1}\boxed{00}(10}_{})^{d+1}}^{\text{reflect}}(01)^{e+1}) \leftrightarrow I((\underbracket{01)^{d+1}\boxed{00}(10)^{c+1}(01)^{b+1}(1}_{}\,0)^{a+1}(01)^{e+1}).$$

However, other integrals of (Type 1) cancel with further integrals of (Type 1), and some permutation of the a_i. Namely

$$I((01)^{a+1}(10)^{b+1}\overbrace{(\underbracket{0\,1)^{c+1}\boxed{00}(10}_{})^{d+1}}^{\text{reflect}}(01)^{e+1}) \leftrightarrow I((01)^{a+1}(10)^{b+1}(\underbracket{01)^{d+1}\boxed{00}(1}_{}\,0)^{c+1}(01)^{e+1})\,.$$

Similarly, integrals of (Type 4) and (Type 5) cancel, by duality. The sum over all weak compositions includes all permutations of the individual a_i, so this cancellation is okay.

If a subsequence ends at the end of $\boxed{00}$, or starts at the start of $\boxed{00}$, then it can be made to cancel by reflecting the blocks containing the subsequence. For example

$$I((01)^{a+1}(10)^{b+1}\overbrace{(\underbracket{0\,1)^{c+1}\boxed{00}}_{}(10)^{d+1}}^{\text{reflect}}(01)^{e+1}) \leftrightarrow I((01)^{a+1}(10)^{b+1}(01)^{d+1}\underbracket{\boxed{00}(1}_{}\,0)^{c+1}(01)^{e+1})$$

shows how some (Type 1) integrals cancel with other (Type 1) integrals, for some permutation of the a_i. This example

$$I(\overbrace{(\underbracket{0\,1)^{a+1}(10)^{b+1}(01)^{c+1}\boxed{00}}_{}(10)^{d+1}}^{\text{reflect}}(01)^{e+1}) \leftrightarrow I((01)^{d+1}\underbracket{\boxed{00}(10)^{c+1}(01)^{b+1}(1}_{}\,0)^{a+1}(01)^{e+1})$$

shows how some (Type 1)integrals cancel with (Type 2) integrals, for some permutation of the a_i. An analogous cancellation holds for (Type 4) and (Type 5) integrals by duality.

So far all of the cancellation has happened by using the usual technique of reflecting the blocks containing the subsequence. Unfortunately, this cannot be used to cancel the last remaining subsequences. The remaining subsequences we must consider begin, or end, at the midpoint of $\boxed{00}$ or $\boxed{11}$. They may also go to the end points of the (Type 3) integral.

We can cancel these subsequences on (Type 2) and (Type 3) integrals, with some permutation of the a_i as follows

$$I((01)^{a+1}\boxed{0}\overbrace{\underbrace{\boxed{0}(10)^{b+1}}_{}(01)^{c+1}(10)^{d+1}(01)^{e+1}}^{\text{reflect}}) \leftrightarrow I(\boxed{0}(10)^{a+1}(01)^{e+1}(10)^{d+1}\underbrace{(01)^{c+1}(10)^{b+1}\boxed{1}}_{}) \,.$$

And by duality, these subsequences on (Type 4) and (Type 3), with some permutation of the a_i will also cancel.

Attempting to cancel by reflecting the blocks for the subsequence

$$I((01)^{a+1}\overbrace{\underbrace{(10)^{b+1}(01)^{c+1}\boxed{0}}_{}}^{\text{reflect}}\boxed{0}(10)^{d+1}(01)^{e+1})$$

leads to the subsequence

$$I((01)^{a+1}\underbrace{\boxed{1}(01)^{c+1}(10)^{b+1}}_{}\boxed{0}(10)^{d+1}(01)^{e+1}) \,.$$

But this is not an integral of (Type 1)–(Type 5), since the odd length blocks are no longer consecutive! Instead, we may cancel the subsequences on (Type 1) integrals as follows

$$I((01)^{a+1}(10)^{b'}\overbrace{\underbrace{(10)^{b''}(01)^{c+1}\boxed{0}}_{}\boxed{0}(10)^{d+1}(01)}^{\text{reflect}}(01)^{e})$$

$$\updownarrow$$

$$I((01)^{a+1}(10)^{b'}\overbrace{\underbrace{(10)(01)^{d+1}\boxed{0}}_{}\boxed{0}(10)^{c+1}(01)^{b'}}^{\text{reflect}}(01)^{e}) \,.$$

In this case an integral of (Type 1) with lengths a_i given by (a, b, c, d, e), cancels with an integral (Type 1)with lengths a_i given by $(a, b', d, c, b'' + e - 1)$, where $b' + b'' = b + 1$. These are two different *compositions*, which are not just related by a permutation. A similar cancellation happens with (Type 5) integrals, by duality. By summing over all weak compositions of the parameters a_i, we can guarantee that this cancellation is okay.

Therefore, if we sum over all weak compositions of the parameters a_i, we deduce that all terms in $D_{<N}$ cancel. By Brown's characerisation of $\ker D_{<N}$, from Theorem 1.2.15, we have that this sum is in $\pi^{\mathrm{wt}}\mathbb{Q}$. □

Remark 2.7.14. More generally it appears that

$$\sum_{\substack{a_1+\cdots+a_{2n+3}=m \\ a_i \geq 0}} \zeta_{\mathcal{C}}(\{1,3\}^n, 3, 3 \mid a_1, \ldots, a_{2n+3}) \in \pi^{\mathrm{wt}}\mathbb{Q}$$

is motivically provable. The proof should be obtained by appropriately generalising the above proof.

It appears that one can also give other curious motivically provable symmetrisations for the $\zeta_{\mathcal{C}}(1,3,3,3 \mid 0,0,0,0,n)$ identity, and others of a similar form. These symmerisations involve a sum taken over a very specific lists of compositions. One example of this is the following.

$$\begin{aligned}&\zeta_{\mathcal{C}}(1,3,3,3 \mid 0,0,0,0,n) + \zeta_{\mathcal{C}}(1,3,3,3 \mid 0,0,0,n,0) + \\ &\quad + \sum_{i=1}^{n-2} \zeta_{\mathcal{C}}(1,3,3,3 \mid 0,0,i,0,n-i) + \\ &\quad + \zeta_{\mathcal{C}}(1,3,3,3 \mid 0,1,0,n-1,0) \overset{1}{=} (n+1)\frac{\pi^{\mathrm{wt}}}{(\mathrm{wt}+1)!}\end{aligned}$$

I do not yet know how this fits into the above framework of generating motivically provable identities, but it suggests that there may be more general ways to cancel terms in $D_{<N}$.

Remark 2.7.15. By incorporating the new types of cancellation introduced in the above proof, and any types of cancellation arising from the above remark, it may be possible to obtain a more general framework for proving motivic identities and generalising Theorem 2.3.8.

2.8 Numerically found block relations, and ranks of relations

In this final section, we would like to mention a number of numerically found identities which can be expressed rather neatly using the block decomposition. This is very much in the spirit of the original cyclic insertion conjecture paper [BBBL98]. We will also indicate what fraction of the MZV relations are obtained by these identities and the cyclic insertion identities.

2.8.1 Other block relations

Notation 2.8.1. We will use the notation $\mathrm{Alt}_{\{\, x_1,\ldots,x_n \,\}}$ to mean the signed sum over all permutation of the variables x_i. That is

$$\mathrm{Alt}_{\{\, x_1,\ldots,x_n \,\}} f(x_1,\ldots,x_n) \coloneqq \sum_{\sigma\in S_n} \mathrm{sgn}(\sigma) f(x_{\sigma(1)},\ldots,x_{\sigma(n)})$$

In Section 7.2 of the paper [BBBL98], the authors mention that the following identity, distinct from the cyclic insertion conjecture, appears to hold.

$$\mathrm{Alt}_{\{\, a_1,a_3,a_5 \,\}} \zeta(1,3,1,3 \mid a_1,a_2,a_3,a_4,a_5) \overset{?}{=} 0\,.$$

What is not to be remarked on, is that this identity appears to readily generalise to the following

$$\mathrm{Alt}_{\{\, a_i \,\mid\, i \text{ odd} \,\}} \zeta(\{1,3\}^n \mid a_1,\ldots,a_{2n+1}) \overset{?}{=} 0\,. \tag{2.8.1}$$

We can try to convert these to block decompositions. In this case, Equation 2.8.1 reads

$$\mathrm{Alt}_{\{\, a_i \,\mid\, i \text{ odd} \,\}} I_{\mathrm{bl}}(2a_1+2, 2a_2+2,\ldots,2a_{2n+1}+2) \overset{?}{=} 0\,.$$

From here it is not too much of a leap to see if arbitrary block lengths work. Indeed we get

Conjecture 2.8.2 (Alternating odd position blocks). *Let $I_{\mathrm{bl}}(\ell_1, \ldots, \ell_{2n+1})$ be a block decomposition of an even weight integral with > 1 block. We have*

$$\mathrm{Alt}_{\{\, \ell_i \,\mid\, i \; odd \,\}} I_{\mathrm{bl}}(\ell_1, \ldots, \ell_{2n+1}) \overset{?}{=} 0 \,.$$

Conjecture-Example 2.8.3. Consider applying Conjecture 2.8.2 to

$$\begin{aligned} z &= \zeta(\{3\}^{2n-1}, (1,2) \mid a_1, \ldots, a_{2n+1}) \\ &= \pm I_{\mathrm{bl}}(2a_1 + 3, 2a_2 + 3, \ldots, 2a_{2n-2} + 3, 2a_{2n} + 2, 2a_{2n+1} + 3) \,. \end{aligned}$$

The only even block length $2a_{2n} + 2$ occurs in position $2n$. Since the sum is taken over permutations of the odd positions, this length is unchanged. Therefore every permutation in the sum expresses the same type of MZV as z.

We obtain

$$\mathrm{Alt}_{\{\, a_i \,\mid\, i \text{ odd} \,\}} \zeta(\{3\}^{2n-1}, (1,2) \mid a_1, \ldots, a_{2n+1}) \overset{?}{=} 0 \,.$$

This can be numerically verified in various cases.

Remark 2.8.4. Various other relations appear to hold, which can be described using the block decomposition. For example

$$\mathrm{Alt}_{\{\, a_1, a_2, a_3 \,\}} \sum_{C_7} I_{\mathrm{bl}}(1, 1, a_1, 1, a_2, n, a_3) \overset{?}{=} 0 \,.$$

Notice the inner sum looks like a cyclic insertion sum. However, since there are two consecutive blocks $\ell_1 = \ell_2 = 1$, Conjecture 2.5.1 does not apply.

Currently these relations are not well structured, having been found in a very ad-hoc manner. Further investigation may identify larger patterns, and a more overarching structure.

Remark 2.8.5. Notice that in the case of 3 blocks, Conjecture 2.8.2 simply expresses the duality of iterated integrals, as explained in Remark 2.2.16

2.8.2 Ranks of relations

Finally, it is worth considering what fraction of MZV relations we get from these identities: the cyclic insertion identities Conjecture 2.5.1, the symmetric insertion identities Theorem 2.5.4, and even the alternating sum identities Conjecture 2.8.2.

Symmetric and Cyclic: Consider weight t, and furthermore assume t is even. We first consider how to obtain equations from cyclic and symmetric insertion, which are not trivially linearly dependent.

Let $c = [\ell_1, \ldots, \ell_{2n+1}]$ be a composition of t into an odd number > 1 of parts, with each part $\ell_i \geq 1$. Since the composition with 1 part gives a tautologically true identity, we ignore it.

If c contains no consecutive $\ell_i = \ell_{i+1}$, then c gives rise to a cyclic insertion identity. If c does not contain two length one blocks $\ell_i = \ell_j = 1$, then the sum over all permutations is redundant because it breaks up into cyclic insertion sums. Otherwise, some permutation of c contains a consecutive $\ell_i = \ell_{i+1}$ and cyclic insertion doesn't apply, so we should also compute the symmetric sum for c.

Weight	Number of cyclic	Number of symmetric	Rank of cyclic and symmetric	Expected number of relations $2^{k-2} - d_k$
4	3	2	3	3
6	7	5	11	14
8	22	10	31	60
10	62	20	81	249
12	181	37	217	1012
14	535	66	600	4075
16	1614	113	1726	16347

From the table it appears the rank of the cyclic and symmetric relations is simply

$$\text{rank(cyclic and symmetric)} = \#\text{cyclic} + \#\text{symmetric} - 1\,.$$

Unless this is prevented by the total number of relations $2^{k-2} - d_k$

Alternating: We now consider how to obtain non-trivial equations from the alternating sum identities, Conjecture 2.8.2. We will restrict ourselves to identities from > 3 blocks. The conjecture does not apply in the case of 1 block, and in the case of 3 blocks it is simply the duality relation.

If any of the odd positions in the composition c are repeated, then the terms in the alternating sum identity will trivially cancel to 0. This is because a transposition of these blocks changes the sign of the summand. Therefore discount these compositions from the list.

Weight	Number of alternating	Rank of alternating	Expected number of relations $2^{k-2} - d_k$
4	0	0	3
6	1	1	14
8	7	7	60
10	25	25	249
12	68	68	1012
14	161	161	4075
16	351	351	16347

From the table it appears that the alternating relations are always linearly independent.

Both and duality: Lastly, we consider how these sets of relations interact, and how many new relations they give on top of the duality of MZV's.

Weight	Rank of alternating, cyclic and symmetric	Rank of Duality	Rank of duality, alternating, cyclic and symmetric	Expected number of relations $2^{k-2} - d_k$
4	3	1	3	3
6	12	6	13	14
8	38	28	50	60
10	105	120	181	249
12	282	496	657	1012
14	755	2016	2436	4075
16	2066	8128	9247	16347

On top of duality, the relations given by the cyclic, symmetric and alternating sum do not add a *significant* number of new relations. By themselves, the cyclic, symmetric and alternating sum relations appear to be largely independent, and do produce plenty of relations. The discovery of further families of block relations, as mentioned above, may help close the gap with the expected number of relations on MZV's.

Chapter 3

Multiple polylogarithms, the coproduct and the symbol

In this chapter we review the definitions and theory surrounding polylogarithms and multiple polylogarithms (MPL's). The definition (Definition 3.1.1) of the polylogarithm $\mathrm{Li}_n(x)$ is motivated by generalising the Taylor series of $-\log(1-x)$. By considering products of polylogarithms, we are lead naturally to multiple polylogarithms (Definition 3.1.2), and then see how to write MPL's as iterated integrals (Theorem 3.1.5). Some reasons for interest in MPL's are discussed, particularly the existence of functional equations (Section 3.2) for $\mathrm{Li}_n(x)$ which play an important role in K-theory and particle physics calculations.

Next we introduce the symbol of an MPL (Section 3.3). This is an algebraic object which contains information about the analytic and differential properties of an MPL, and is an important tool for finding both functional equations and relations between MPL's. We review Goncharov's tree definition (Section 3.3.1) of the symbol (called the $\otimes^m$-invariant, Definition 3.3.4), and see the connection with iterating the coproduct (Section 3.3.2) on his Hopf algebra of motivic iterated integrals. We also look at the differential interpretation (Section 3.3.3) of the symbol, and its connection with the differential forms appearing in iterated integrals. We also review Gangl, Goncharov and Levine's polygon algebra and Rhodes's hook-arrow trees (Section 3.3.4), and their connection with the symbol. We also mention the Mathematica implementation in Duhr's PolylogTools package [PT].

Finally we consider the different 'levels' of information which can be extracted from the symbol by looking modulo products (Section 3.4.1), or looking modulo products and depth 1 terms ("modulo δ" Section 3.4.2). We see also that Nielsen polylogarithms provide an 'obstruction' to the rule of thumb that a symbol vanishing modulo δ can be written in terms of Li_n's (Section 3.4.2.1).

3.1 Definition of polylogarithms and multiple polylogarithms

The s-th polylogarithm function is a generalisation of the usual logarithm function $\log(z)$, motivated by considering the Taylor series of $-\log(1-z)$.

The Taylor series of $-\log(1-z)$ is

$$-\log(1-z) = \sum_{n=1}^{\infty} \frac{z^n}{n} \,.$$

The exponent of n in the denominator is n^1, so we make the following generalisation to define the polylogarithms as first done by Leibniz [Lei55].

Definition 3.1.1 (Polylogarithm)**.** For $s \in \mathbb{Z}_{>0}$, the s-th polylogarithm function $\mathrm{Li}_s(z)$ is defined by the following Taylor series

$$\mathrm{Li}_s(z) \coloneqq \sum_{n=1}^{\infty} \frac{z^n}{n^s} \quad , \, |z| < 1 \,.$$

By taking $s = 1$, we find that

$$\mathrm{Li}_1(z) = -\log(1-z) \,,$$

so we recover the usual logarithm, and $\mathrm{Li}_s(z)$ genuinely does generalise it.

By computing the derivative of $\mathrm{Li}_s(z)$, one finds

$$\frac{\mathrm{d}}{\mathrm{d}z} \mathrm{Li}_s(z) = \mathrm{Li}_{s-1}(z) \,,$$

so one can analytically continue $\mathrm{Li}_s(z)$ to the cut complex plane $\mathbb{C} \setminus [1, \infty)$ by the following integral

$$\mathrm{Li}_s(z) = \int_0^z \mathrm{Li}_{s-1}(t) \frac{\mathrm{d}t}{t} \,.$$

In the same way that multiple zeta values can be motivated by considering products of Riemann zeta values (see Section 1.1.1), one can motivate and define a *multiple* polylogarithm as in [Gon95b]. Henceforth "multiple polylogarithm" may be abbreviated as MPL.

Definition 3.1.2 (Multiple polylogarithm)**.** Let $s_i \in \mathbb{Z}_{>0}$, then the multiple polylogarithm function $\mathrm{Li}_{s_1,\ldots,s_k}(z_1, \ldots, z_k)$ is defined by the following series

$$\mathrm{Li}_{s_1,\ldots,s_k}(z_1, \ldots, z_k) \coloneqq \sum_{0<n_1<n_2<\cdots<n_k} \frac{z_1^{n_1} \cdots z_k^{n_k}}{n_1^{s_1} \cdots n_k^{s_k}} \,.$$

For example, by considering the product $\mathrm{Li}_s(x) \,\mathrm{Li}_t(y)$, we obtain

$$\mathrm{Li}_s(x) \,\mathrm{Li}_t(y) = \sum_{n,m=1}^{\infty} \frac{x^n y^m}{n^s m^t} \,.$$

We can then break the sum over $n, m = 1$ to ∞ into $n < m$, $n = m$, and $n > m$, to get

$$\begin{aligned} &= \left(\sum_{n<m} + \sum_{n=m} + \sum_{n>m} \right) \frac{x^n y^m}{n^s m^t} \\ &= \mathrm{Li}_{s,t}(x, y) + \mathrm{Li}_{s+t}(xy) + \mathrm{Li}_{t,s}(y, x) \,. \end{aligned}$$

This is an example of the stuffle product on MPL's, which should be compared with the analogous construction on MZV's in Section 1.1.4.3

Moreover, by taking $z_i = 1$ in the MPL $\mathrm{Li}_{s_1,\ldots,s_k}(z_1,\ldots,z_k)$ we find that

$$\mathrm{Li}_{s_1,\ldots,s_k}(1,\ldots,1) = \zeta(s_1,\ldots,s_k)\,.$$

Therefore, the multiple zeta values of Chapter 1 can be viewed as special values of MPL's, as claimed.

The notions of depth and weight have analogues for MPL's.

Definition 3.1.3 (MPL weight, MPL depth)**.** Given a MPL $\mathrm{Li}_{s_1,\ldots,s_k}(z_1,\ldots,z_k)$, we make the following definitions.

- The sum of the indices $s_1 + \cdots + s_k$ is called the weight of $\mathrm{Li}_{s_1,\ldots,s_k}(z_1,\ldots,z_k)$.
- The number k of its indices is called the depth of $\mathrm{Li}_{s_1,\ldots,s_k}(z_1,\ldots,z_k)$.

3.1.1 Multiple polylogarithms as iterated integrals

One viewpoint that we will make continual use of in the rest of this thesis is the equivalence between multiple polylogarithms and certain iterated integrals. Recall the definition of an iterated integral from Definition 1.1.10 in Section 1.1.3.

The iterated integral

$$I_\gamma(x_0; x_1,\ldots,x_m; x_{m+1}) = \int_\gamma \omega(x_1)\circ\cdots\circ\omega(x_m)\,,$$

γ a path from x_0 to x_{m+1}, is sometimes referred to as a *multiple logarithm* [Gon98]. It can also called a *hyperlogarithm* [p. 8, Gon01], having been considered by under this name by Kummer [Kum40], Lappo-Danilevsky [LD28], and Poincaré (but as an analytic functions of the upper limit x_{m+1} only, in the case where $x_0 = 0$). Here they are considered as multivalued anlaytic functions of $x_0,\ldots,x_{m+1}$.

Goncharov [Gon98] gives the following definition of a 'multiple polylogarithm' in terms of the above iterated integral.

Definition 3.1.4 (Goncharov multiple polylogarithm)**.** Let $s_i \in \mathbb{Z}_{>0}$, then the multiple polylogarithm $I_{s_1,\ldots,s_k}(z_1,\ldots,z_k)$ is defined by

$$I_{s_1,\ldots,s_k}(z_1,\ldots,z_k) \coloneqq I(0; x_1, \{0\}^{s_1-1},\ldots,x_k,\{0\}^{s_k-1};1)\,.$$

Goncharov's choice to name this $I_{s_1,\ldots,s_k}(z_1,\ldots,z_k)$ a multiple polylogarithm is justified. The functions $I_{s_1,\ldots,s_k}$ and $\mathrm{Li}_{s_1,\ldots,s_k}$ are closely related by the following theorem.

Theorem 3.1.5 (Goncharov, Theorem 2.2 in [Gon01])**.** *Suppose $|z_i| < 1$, for all z_i. The functions $\mathrm{Li}_{s_1,\ldots,s_k}$ and $I_{s_1,\ldots,s_k}$ are related as follows.*

$$\mathrm{Li}_{s_1,\ldots,s_k}(z_1,\ldots,z_k) = (-1)^k I_{s_1,\ldots,s_k}\big(\tfrac{1}{z_1\cdots z_k},\tfrac{1}{z_2\cdots z_k},\ldots,\tfrac{1}{z_k}\big)\,.$$

Proof sketch: For simplicity, Goncharov restricts to the case $k = 2$. This makes the idea of the proof clear, without getting bogged down when keeping track of all of the details for higher depth. Rhodes gives a version of this proof with more details than Goncharov in [Rho12].

In the case $k = 2$, the integral is

$$(-1)^2 \int_{0 \leq t_1 \leq \cdots \leq t_{s_1+s_2} \leq 1} \frac{\mathrm{d}t_1}{t_1 - \frac{1}{x_1 x_2}} \wedge \frac{\mathrm{d}t_2}{t_2} \wedge \cdots \wedge \frac{\mathrm{d}t_{s_1}}{t_{s_1}} \wedge \wedge \frac{\mathrm{d}t_{s_1+1}}{t_{s_1+1} - \frac{1}{x_2}} \wedge \frac{\mathrm{d}t_{s_1+2}}{t_{s_1+2}} \wedge \cdots \wedge \frac{\mathrm{d}t_{s_1+s_2}}{t_{s_1+s_2}}, \tag{3.1.1}$$

and Goncharov claims this is equal to

$$\mathrm{Li}_{s_1,s_2}(x_1, x_2) = \sum_{0<n_1<n_2} \frac{x_1^{n_1} x_2^{n_2}}{n_1^{s_1} n_2^{s_2}}.$$

We can develop

$$\frac{\mathrm{d}t_1}{t_1 - \frac{1}{x_1 x_2}}$$

as a geometric series. We obtain

$$\begin{aligned} &= -(x_1 x_2) \frac{\mathrm{d}t_1}{1 - t_1 x_1 x_2} \\ &= -(x_1 x_2)\, \mathrm{d}t_1 \sum_{i=0}^{\infty} (t_1 x_1 x_2)^i \\ &= -\frac{\mathrm{d}t_1}{t_1} \sum_{i=1}^{\infty} (t_1 x_1 x_2)^i . \end{aligned}$$

Plugging this, and the corresponding result for $\frac{\mathrm{d}t_{s_1+1}}{t_{s_1+1} - \frac{1}{x_2}}$ back into the integral gives

$$= \int_{0 \leq t_1 \leq \cdots \leq t_{s_1+s_2} \leq 1} \frac{\mathrm{d}t_1}{t_1} \sum_{i=1}^{\infty} (t_1 x_1 x_2)^i \wedge \frac{\mathrm{d}t_2}{t_2} \wedge \cdots \wedge \frac{\mathrm{d}t_{s_1}}{t_{s_1}} \wedge \wedge \frac{\mathrm{d}t_{s_1+1}}{t_{s_1+1}} \sum_{j=1}^{\infty} (t_{s_1+1} x_2)^j \wedge \frac{\mathrm{d}t_{s_1+2}}{t_{s_1+2}} \wedge \cdots \wedge \frac{\mathrm{d}t_{s_1+s_2}}{t_{s_1+s_2}} .$$

Now integrate term by term, integrating out the variable t_1 first. We get that

$$\begin{aligned} \int_{0 \leq t_1 \leq t_2} \frac{\mathrm{d}t_1}{t_1} \sum_{i=1}^{\infty} (t_1 x_1 x_2)^i &= \left[\sum_{i=1}^{\infty} \frac{(t_1 x_1 x_2)^i}{i} \right]_{t_1=0}^{t_2} \\ &= \sum_{i=1}^{\infty} \frac{(t_2 x_1 x_2)^i}{i} . \end{aligned}$$

We can repeat this for $t_2, t_3, \ldots, t_{s_1}$, to get that the original integral Equation 3.1.1 equals

$$\begin{aligned} &= \int_{0 \leq t_{s_1+1} \leq \cdots \leq t_{s_1+s_2} \leq 1} \frac{\mathrm{d}t_{s_1+1}}{t_{s_1+1}} \sum_{i=1}^{\infty} \frac{(t_{s_1+1} x_1 x_2)^i}{i^{s_2}} \sum_{j=1}^{\infty} (t_{s_1+1} x_2)^j \wedge \frac{\mathrm{d}t_{s_1+2}}{t_{s_1+2}} \wedge \cdots \wedge \frac{\mathrm{d}t_{s_1+s_2}}{t_{s_1+s_2}} \\ &= \int_{0 \leq t_{s_1+1} \leq \cdots \leq t_{s_1+s_2} \leq 1} \frac{\mathrm{d}t_{s_1+1}}{t_{s_1+1}} \sum_{i,j=1}^{\infty} \frac{x_1^i}{i^{s_1}} (t_{s_1+1} x_2)^{i+j} \wedge \frac{\mathrm{d}t_{s_1+2}}{t_{s_1+2}} \wedge \cdots \wedge \frac{\mathrm{d}t_{s_1+s_2}}{t_{s_1+s_2}} . \end{aligned}$$

Then integrate out $t_{s_1+1}, \ldots, t_{s_1+s_2}$ in the same way to get

$$= \sum_{i,j=1}^{\infty} \frac{x_1^i x_2^{i+j}}{i^{s_1}(i+j)^{s_2}} .$$

Finally, we can make the change of variables $\ell = i + j$. The new summation range runs over $0 < i < \ell$, so the sum becomes

$$= \sum_{0<i<\ell} \frac{x_1^i x_2^\ell}{i^{s_1}\ell^{s_2}} = \mathrm{Li}_{s_1,s_2}(x_1, x_2) ,$$

as claimed. □

Remark 3.1.6. In the case where $z_1 = \cdots = z_k = 1$, we obtain that

$$\zeta(s_1, \ldots, s_k) = (-1)^k I_{s_1,\ldots,s_k}(1, \ldots, 1) = (-1)^k I(0; 1, \{0\}^{s_1-1}, \ldots, 1, \{0\}^{s_k-1}; 1) ,$$

which finally completes the proof of Proposition 1.1.16.

3.1.2 Variants and modified polylogarithms

The polylogarithm Li_n is a multivalued analytic function on $\mathbb{C} \setminus \{ 0, 1 \}$. However, there is an associated single-valued version, defined as follows.

Definition 3.1.7 (Single-valued polylogarithm, [Zag91])**.** For $n \geq 1$, define the single valued polylogarithm $\mathscr{L}_n$ as follows.

$$\mathscr{L}_n(z) \coloneqq \mathrm{Re}_n \left(\sum_{k=0}^{n} \frac{B_k 2^k}{k!} \log|z| \, \mathrm{Li}_{n-k}(z) \right) , \quad n \geq 2$$
$$\mathscr{L}_1(z) \coloneqq \log|z| ,$$

where B_k are the Bernoulli numbers defined in Definition 1.1.5, and

$$\mathrm{Re}_n \coloneqq \begin{cases} \mathrm{Re} & \text{if } n \text{ odd} \\ \mathrm{Im} & \text{if } n \text{ even.} \end{cases}$$

These functions will play a role when describing functional equations of polylogarithms; essentially $\mathscr{L}_n$ satisfies 'clean' functional equations, without any lower order product terms. Moreover, they enter into an important conjecture on special values of the Dedekind zeta function [Section 8 in Zag91].

Zagier proved that $\mathscr{L}_n(z)$ is real-analytic on $\mathbb{C} \setminus \{ 0, 1 \}$. More precisely

Theorem 3.1.8 (Zagier, [Zag91])**.** *The function $\mathscr{L}_n(z)$ is single-valued and continuous on $\mathbb{P}^1(\mathbb{C})$.*

3.2 Functional equations for polylogarithms

The big area of interest with regard to polylogarithms is in finding and understanding their functional equations. There are at least two reasons for this interest. On the number theory side, polylogarithms have a role as 'higher regulators' of a number field, and sufficiently generic functional equations for Li_n should play some role in giving explicit generators and relations for the K-groups $K_{2n+1}(F)$. This in turn feeds into Zagier's conjecture on special values of the Dedekind zeta function [Zag91]. Roughly: up to known factors, $\zeta_F(n)$ can be expressed as an $r_2(F) \times r_2(F)$ determinant of $\mathscr{L}_n$'s of elements of F. The case $\zeta_F(2)$ was partially handled by Zagier [Zag86] using a connection to volumes of hyperbolic manifolds. Generally it follows from the work of Bloch and Suslin [Blo77; Sus86]. The case $\zeta_F(3)$ was proven by Goncharov [Gon91] using his Li_3 functional equation.

On the physics side, calculations of amplitudes and Feynman integrals often produce large expressions involving polylogarithms and MPL's [RV00; Wei07; BW11]. For example, the full analytic expession for the remainder function for the 'two-loop Hexagon Wilson loop' $R^{(2)}_{6,WL}$ involves weight 4 multiple polylogarithms, and fills 17 pages of appendix H in [DDDS10]. Having a good understanding of (multiple) polylogarithm functional equations can lead to drastically simpler formulae, both in terms of length and in terms of the complexity of the functions involved. In [GSVV10], this remainder function $R^{(2)}_{6,WL}$ was re-written as a *single* line of classical Li_4 polylogarithms after observing the vanishing of the symbol of $R^{(2)}_{6,WL}$ modulo δ, where δ is as in Section 3.4.2 below.

3.2.1 Examples of functional equations

The baby instance of polylogarithm functional equations comes from the fundamental property of log, namely $\log(xy) = \log(x) + \log(y)$. In terms of $\mathrm{Li}_1(x)$ we have the following.

Proposition 3.2.1. *The polylogarithm* Li_1 *satisfies the following functional equation*

$$\mathrm{Li}_1(1 - xy) = \mathrm{Li}_1(1 - x) + \mathrm{Li}_1(1 - y)\,.$$

Proof. This is just a direct application of the definition that $\mathrm{Li}_1(x) = -\log(1 - x)$, and the functional equation $\log(xy) = \log(x) + \log(y)$. ☐

This is expected to be a feature of all higher weight polylogarithms. Indeed every polylogarithm satisfies its own version of the so-called duplication relation, or the more general so-called distribution relations.

Proposition 3.2.2 (Distribution relation, duplication relation)**.** *Let* $\zeta_p \coloneqq \exp(2\pi \mathrm{i}/p)$ *be a primitive* p*-th root of unity,* $p \in \mathbb{Z}_{>0}$*. Then* Li_k *satisfies the following functional equation*

$$\mathrm{Li}_k(x^p) = p^{k-1} \sum_{j=0}^{p-1} \mathrm{Li}_k(\zeta_p^j x)\,.$$

This reduces to the so-called duplication relation

$$\mathrm{Li}_k(x^2) = 2^{k-1} \left(\mathrm{Li}_k(x) + \mathrm{Li}_k(-x)\right)$$

in the case $p = 2$*.*

Proof. Write out the Taylor series for both sides. On the right hand side we get

$$p^{k-1} \sum_{n=1}^{\infty} \frac{\sum_{j=0}^{p-1} (\zeta_p^j x)^n}{n^k} \, .$$

When $p \mid n$, the numerator becomes px^n since each term $(\zeta_p^j)^n$ is identically 1. Otherwise the numerator is 0 since ζ_p^n is another primitive p-th root, and we just get some permutation of

$$\sum_{j=0}^{p-1} \zeta_p^j = \frac{\zeta_p^p - 1}{\zeta_p - 1} = 0 \, .$$

Only the term $p \mid n$ survive, so we can take $n = pm$ on the right hand side, and get

$$= p^{k-1} \sum_{m=1}^{\infty} \frac{px^{mp}}{(mp)^k} = \sum_{m=1}^{\infty} \frac{(x^p)^m}{m^k} = \mathrm{Li}_k(x^p) \, ,$$

as claimed. □

The duplication relations, the distribution relations, and the so-called inversion relations

$$\mathrm{Li}_k(z) + (-1)^k \mathrm{Li}_k\left(\frac{1}{z}\right) = \text{ elementary}$$

are considered *trivial*. They can be proven easily for polylogarithms of any weight, and so are not particularly interesting.

Beyond these trivial functional equations, it is expected that every polylogarithm satisfies some non-trivial function equations, but so far these are only know up to Li_7 [Gan03]. The prototypical example of such a non-trivial functional equation is the 5-term relation for the dilogarithm (weight 2 polylogarithm). This functional equation has been discovered and re-discovered many times by many different people including Abel, Spencer, Kummer, Hill and Schaeffer.

Theorem 3.2.3 (5-term relation, Schaeffer's [Sch46] form of Abel's equation [Abe81, p. 193])**.** *The polylogarithm* Li_2 *satisfies the following functional equation. For* $0 < y < x < 1$*, we have*

$$\begin{aligned} &\mathrm{Li}_2(x) - \mathrm{Li}_2(y) + \mathrm{Li}_2\left(\frac{y}{x}\right) - \mathrm{Li}_2\left(\frac{1-1/x}{1-1/y}\right) + \mathrm{Li}_2\left(\frac{1-x}{1-y}\right) \\ &= \frac{\pi^2}{6} - \log(x)\log\left(\frac{1-x}{1-y}\right) \end{aligned}$$

Written in terms of the modified polylogarithm $\mathscr{L}_2(z)$ above, the 5-term relation simplifies to the following

$$\mathscr{L}_2(x) - \mathscr{L}_2(y) + \mathscr{L}_2\left(\frac{y}{x}\right) - \mathscr{L}_2\left(\frac{1-1/x}{1-1/y}\right) + \mathscr{L}_2\left(\frac{1-x}{1-y}\right) = 0 \, .$$

This illustrates what was meant earlier by saying $\mathscr{L}_n$ satisfies 'clean' functional equations, without any extra product terms.

The 5-term relation for Li_2 is expected to be the fundamental functional equation for Li_2, in the sense that every other functional equation follows by specialising it, but currently this remains only a conjecture. Some evidence in this direction can be see in [Sou15] , where an infinite family of dilogarithm functional equations (arising from the combinatorics of dihedral coordinates on $\mathfrak{M}_{0,n}$) is proven to reduce to 5-term relations. Other evidence come from Wojtkowiak's result [Woj96] that every one variable functional equation for Li_2 can be obtained by specialising the 5-term relation.

Moreover, it is known, that the 5-term relation somehow characterises the dilogarithm in the sense that any measurable function $f(z)$, $z \in \mathbb{C}$ that satisfies the 5-term relation is proportional to $\mathscr{L}_2(z)$ [Blo00].

3.2.2 Geometry behind polylogarithm functional equations

Functional equation for Li_2: The 5-term relation for Li_2 can be described elegantly in terms of the geometry of the projective line $\mathbb{P}^1(\mathbb{C})$. This motivates a search for functional equations arising from geometric constructions.

Recall the cross-ratio of 4 points $z_1, \ldots, z_4 \in \mathbb{C}$ is defined by

$$\mathrm{cr}(z_1, z_2; z_3, z_4) \coloneqq \frac{z_1 - z_3}{z_1 - z_4} \Big/ \frac{z_2 - z_3}{z_2 - z_3} \,.$$

By using the homogeneous coordinates of $\mathbb{P}^1(\mathbb{C})$, and writing $Z_i = [1 \colon z_i]$, the cross-ratio can be defined on all of $\mathbb{P}^1(\mathbb{C}) = \mathbb{C} \cup \{ \infty \}$.

The 5-term relation for Li_2 now has the following form. Let $z_1, \ldots, z_5$ be 5 points in $\mathbb{P}^1(\mathbb{C})$. Then

$$\sum_{i=1}^{5} (-1)^i \mathscr{L}_2(\mathrm{cr}(z_1, \ldots, \widehat{z_i}, \ldots, z_5)) = 0 \,.$$

Taking $z_1 = \infty$, $z_2 = 0$, $z_3 = 1$, $z_4 = x$ and $z_5 = y$ reduces this equation to the previous version of the 5-term relation (up to applying the inversion relation $\mathscr{L}_2(z) = -\mathscr{L}_2(\frac{1}{z})$ to some terms).

Functional equation for Li_3: Goncharov [Gon95a] has exploited this geometric viewpoint to produce a highly generic functional equation for Li_3 using the so-called triple-ratio r_3. He has also produced precise conjectures for what to expect at higher weight, although so far an equivalent Li_4 functional equation has not been found.

Let $\ell_1, \ldots, \ell_7$ be 7 points in $\mathbb{P}^2(\mathbb{C})$, and let $L_i \in \mathbb{C}^3$ be the vector projecting to ℓ_i.

Definition 3.2.4 (Triple-ratio)**.** The triple-ratio of 6 generic points $\ell_1, \ldots, \ell_6$ in $\mathbb{P}^2(\mathbb{C})$ is defined to be the formal linear combination in $\mathbb{Z}[\mathbb{C} \setminus \{ 0, 1 \}]$

$$r_3(\ell_1, \ldots, \ell_6) \coloneqq \frac{1}{15} \mathrm{Alt}_{\{ 1, \ldots, 6 \}} \left[\frac{\Delta(L_1, L_2, L_4)\Delta(L_2, L_3, L_5)\Delta(L_3, L_1, L_6)}{\Delta(L_1, L_2, L_5)\Delta(L_2, L_3, L_6)\Delta(L_3, L_1, L_4)} \right] .$$

Here $\Delta(L_1, L_2, L_3) = \det(L_1 \mid L_2 \mid L_3)$ is the determinant of the matrix with columns L_1, L_2, L_3.

The fully symmetric $840 = 7!/6$-term functional equation [Gon94] is given by

$$\sum_{i=1}^{7} (-1)^i \mathscr{L}_3(r_3(\ell_1, \ldots, \widehat{\ell_i}, \ldots, \ell_7)) = 0 \,.$$

Notation 3.2.5. We will use the notation $\mathrm{Cyc}_{\{\, x_1,\dots,x_n \,\}}$ to mean the sum over all cyclic shifts of the variables x_i. That is

$$\mathrm{Cyc}_{\{\, x_1,\dots,x_n \,\}} f(x_1,\dots,x_n) \coloneqq \sum_{i=1}^{n} f(x_i,\dots,x_n,x_1,\dots,x_{i-1})\,.$$

This triple-ratio can be extended to degenerate configurations of points. For the following highly degenerate choice of points, where ℓ_i is given by the i-th column of the matrix

$$\begin{pmatrix} 1 & 0 & 0 & 1 & 1 & 0 & z \\ 0 & 1 & 0 & 1 & x & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & y & 0 \end{pmatrix},$$

one obtains Goncharov's 22(+1)-term Li_3 functional equation below.

$$\begin{aligned} \mathscr{L}_3(-xyz) + \mathrm{Cyc}_{\{\, x,y,z \,\}} \Bigg\{ & \mathscr{L}_3(zx - x + 1) + \mathscr{L}_3\left(\frac{zx-x+1}{zx}\right) - \mathscr{L}_3\left(\frac{zx-x+1}{z}\right) + \\ & + \mathscr{L}_3\left(\frac{x(yz-z+1)}{-(zx-x+1)}\right) + \mathscr{L}_3(z) + \mathscr{L}_3\left(\frac{yz-z+1}{y(zx-x+1)}\right) + \\ & - \mathscr{L}_3\left(\frac{yz-z+1}{yz(zx-x+1)}\right) \Bigg\} = 3\,\mathscr{L}_3(1) \end{aligned}$$

3.2.3 Bloch groups; towards the symbol of polylogarithms

An important collection of objects that arise when trying to study polylogarithms over $\mathbb{C}$, or more general fields F, are the so-called Bloch groups $\mathcal{B}_n(F)$. They are defined in such a way as to capture, non-explicitly, all of the functional equations of the polylogarithm $\mathscr{L}_n$. In some sense they can be seen as a precursor to the symbol of MPL's.

3.2.3.1 The subgroups of relations $\mathcal{R}_n(F)$

The key to defining the Bloch groups is somehow capturing the functional equations of polylogarithms, despite not being able to explicitly write them all down.

Define by induction subgroups $\mathcal{R}_n(F) < \mathbb{Z}[\mathbb{P}^1(F)]$. Then set

$$\mathcal{B}_n(F) \coloneqq \mathbb{Z}[\mathbb{P}^1(F)] / \mathcal{R}_n(F)$$

to be the weight n *Bloch group*. We will write $\{x\}_n$ for the image of $[x]$ in $\mathcal{B}_n(F)$.

Subgroup $\mathcal{R}_1(F)$: The subgroup $\mathcal{R}_1(F)$ is explicitly defined by

$$\mathcal{R}_1(F) \coloneqq \{\, [x] + [y] - [xy] \mid x, y, \in F^* \,\} \cup \{\, [0], [\infty] \,\}\ .$$

This subgroup $\mathcal{R}_1(F)$ captures the functional equation $\log(xy) = \log(x) + \log(y)$, which we know $\mathscr{L}_1(z) \coloneqq \log|z|$ satisfies.

Inductive definition of $\mathcal{R}_n(F)$: Define a homomorphism δ_n, as follows.

$$\mathbb{Z}[\mathbb{P}^1(F)] \to \begin{cases} \mathcal{B}_{n-1}(F) \otimes F^* & n \geq 3 \\ \bigwedge^2 F^* & n = 2 \end{cases}$$

$$[x] \mapsto \begin{cases} \{x\}_{n-1} \otimes x & n \geq 3 \\ (1-x) \wedge x & n = 2 \end{cases} .$$

Also $\delta \colon [\infty], [0], [1] \mapsto 0$.

Now set

$$\mathcal{A}_n(F) \coloneqq \ker \left(\delta_n \colon \mathbb{Z}[\mathbb{P}^1(F)] \to \begin{cases} \mathcal{B}_{n-1}(F) \otimes F^* & n \geq 3 \\ \bigwedge^2 F^* & n = 2 \end{cases} \right) .$$

Extending by linearity means the specialisation homomorphism $t \mapsto t_0$, $t_0 \in F$, gives a map

$$\mathbb{Z}[\mathbb{P}^1(F(t))] \to \mathbb{Z}[\mathbb{P}^1(F)]$$
$$[f_i(t)] \mapsto [f_i(t_0)] .$$

This works even if t_0 is a pole of $f_i(t)$. We can now give the inductive definition of $\mathcal{R}_n(F)$ as follows.

Definition 3.2.6 (Subgroup of relations)**.** The subgroup of relations $\mathcal{R}_n(F)$ is defined by

$$\mathcal{R}_n(F) \coloneqq \{ \, \alpha(0) - \alpha(1) \mid \alpha(t) \in \mathcal{A}_n(F(t)) \, \} \cup \{ \, [0], [\infty] \, \} .$$

3.2.3.2 Consequence for functional equations

By extending $\mathscr{L}(z)$ to $\mathbb{Z}[\mathbb{P}^1(\mathbb{C})]$ by linearity, we obtain the following motivating theorem

Theorem 3.2.7 (Theorem 1.15 in [Gon94])**.**

$$\mathscr{L}_n(\mathcal{R}_n(\mathbb{C})) = 0$$

Which is to say the subspace $\mathcal{R}_n(\mathbb{C})$ does actually give functional equations for $\mathscr{L}_n(z)$.

Sketch of $n = 2$ case: Firstly we need to establish the result of Lemma 1.16 in [Gon94]. Namely for

$$\alpha(t) \coloneqq \sum n_i [f_i(t)] \in \mathbb{Z}[\mathbb{P}^1(\mathbb{C}(t))] ,$$

if

$$0 = \delta_2 \alpha(t) \coloneqq \sum n_i (1 - f_i(t)) \wedge f_i(t) \in \bigwedge^2 \mathbb{C}(t)^* ,$$

then

$$\mathrm{d} \left(\sum n_i \mathscr{L}_2(f_i(z)) \right) = 0 . \tag{3.2.1}$$

It then follows immediately that $\sum n_i \mathscr{L}_2(f_i(z))$ is constant. So $\mathscr{L}_2(\alpha(0) - \alpha(1)) = 0$, and

$$\mathscr{L}_2(\mathcal{R}_2(\mathbb{C})) = 0 .$$

To prove Equation 3.2.1, we need to consider the following diagram.

$$\begin{array}{ccc} \mathbb{Z}[\mathbb{P}^1(\mathbb{C}(t))] & \xrightarrow{\delta_2} & \bigwedge^2 \mathbb{C}(t)^* \\ \big\downarrow \mathscr{L}_2 & & \big\downarrow r_2 \\ S^0(\mathbb{P}^1(\mathbb{C})) & \xrightarrow{\mathrm{d}} & S^1(\mathbb{P}^1(\mathbb{C})) \end{array}$$

Where here

$$r_2(f \wedge g) := -\log|f| \,\mathrm{d}\arg(g) + \log|g| \,\mathrm{d}\arg f\,,$$

and $S^i(\mathbb{P}^1(\mathbb{C}))$ is the space of smooth i-forms on $\mathbb{P}^1(\mathbb{C})$.

Since $\mathscr{L}_2(z) = \mathrm{Im}(\mathrm{Li}_2(z)) + \arg(1-z)\log|z|$, we can compute $\mathrm{d}\mathscr{L}_2(z)$ as follows.

We have

$$\mathrm{d}(\arg(1-z)\log|z|) = \log|z| \,\mathrm{d}\arg(1-z) + \arg(1-z)\,\mathrm{d}\log|z|\,,$$

using the product rule. Also we have

$$\begin{aligned} \mathrm{d}\,\mathrm{Li}_2(z) &= \mathrm{Li}_1(z)\,\mathrm{d}\log(z) \\ &= -\log(1-z)\,\mathrm{d}\log(z) \\ &= -(\log|1-z| + \mathrm{i}\arg z)(\,\mathrm{d}\log|z| + \mathrm{i}\,\mathrm{d}\arg z)\,. \end{aligned}$$

So

$$\mathrm{d}\,\mathrm{Im}(\mathrm{Li}_2(z)) = \mathrm{Im}(\,\mathrm{d}\,\mathrm{Li}_2(z)) = -\log|1-z| \,\mathrm{d}\arg z - \arg(1-z)\,\mathrm{d}\log|z|\;.$$

Overall this means

$$\mathrm{d}\mathscr{L}_2(z) = -\log|1-z| \,\mathrm{d}\arg z + \log|z|\,\mathrm{d}\arg(1-z)\,. \tag{3.2.2}$$

Now Equation 3.2.2 shows that the above diagram in fact commutes. This means that we can make the following computation

$$\begin{aligned} 0 &= r_2 \circ \delta_2(\alpha(t)) \\ &= d \circ \mathscr{L}_2(\alpha(t)) \\ &=: \mathrm{d}\left(\sum n_i \mathscr{L}_2(f_i(z))\right)\,. \end{aligned}$$

This proves the Goncharov's Lemma, and hence proves the theorem for $n = 2$. For the case $n \geq 3$, see [Gon94]. □

This begins to show how powerful the algebraic approach (rather than the analytic approach) to polylogarithms can be. The algebraic object $(1-z) \wedge z$ attached to Li_2 above is closely linked with the symbol of Li_2, to be defined later.

More generally we have the following result of Zagier, moving towards the symbol of Li_n.

Theorem 3.2.8 (Zagier, Proposition 3 in [Zag91])**.** *Let* $\{\, n_i, x_i(t) \,\}$ *be a collection of integers, and rational functions in* $\mathbb{C}(t)$*. Suppose that*

$$\sum n_i [x_i(t)]^{m-2} \otimes ([x_i(t)] \wedge [1 - x_i(t)]) = 0$$

in $(\operatorname{Sym}^{m-2}\mathbb{C}(t)^* \otimes \bigwedge^2 \mathbb{C}(t)^*) \otimes_{\mathbb{Z}} \mathbb{Q}$. *Then*

$$\sum_i n_i \mathscr{L}_m(x_i(t)) = constant\,.$$

That is, the algebraic object $[z]^{m-2} \otimes [z] \wedge [1-z]$ attached to $\mathscr{L}_m(z)$ *detects* functional equations of $\mathscr{L}_m$.

To fit better with the symbol below I would prefer to swap the order of terms over and get $-[1-z] \wedge [z] \otimes [z]^{m-2}$.

3.3 Coproduct, and symbol of MPL's

In this section we will introduce a very important tool for studying the functional equations of MPL's, namely the *symbol*. This tool will be used continually throughout the remainder of this thesis. As hinted at above, the symbol is some algebraic object which can be attached to an MPL, somehow enriching the correspondence $\mathscr{L}_n(x) \leftrightsquigarrow -[1-x] \wedge [x] \otimes [x]^{n-2}$.

The symbol was first introduced by Goncharov, under the name the $\otimes^m$-invariant, in Section 4 of [Gon05]. There it was defined by associating certain combinations of labelled binary trees to the MPL iterated integral $I_{s_1,\ldots,s_k}(x_1,\ldots,x_k)$. Goncharov also identified it as coming from iterating the coproduct on the Hopf algebra of (motivic) iterated integrals.

The symbol should also be seen as somehow describing the differential structure of an MPL. As seen above, t least for $m = 2$, the object $-[1-x] \wedge [x] \otimes [x]^{m-2}$ 'corresponds' to the derivative of $\mathscr{L}_m(x)$. With this viewpoint, it is no so surprising that $\sum n_i[1-x_i(t)] \wedge [x_i(t)] \otimes [x_i(t)]^{m-2} = 0$ leads to $n_i \mathscr{L}_m(x_i(t)) = \text{constant}$. So we ought to expect the symbol of MPL's to play a similar role in detecting and characterising functional equations.

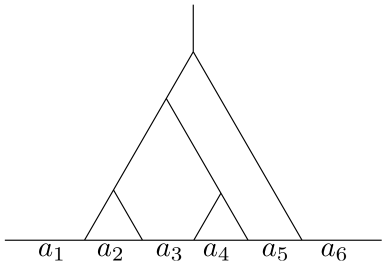
A final viewpoint on the symbol of MPL's is provided by Rhodes's [DGR12; Rho12] hook-arrow tree construction built on top of the polygon algebra of Gangl, Goncharov, and Levin [GGL09]. In Chapter 4 of [Rho12], Rhodes used this construction to give explicit formulae for the symbols of the depth 2 MPL $I_{a,b}(x,y)$ and the depth 3 MPL $I_{a,b,c}(x,y,z)$, for any a,b,c. Duhr is developing this approach into the PolylogTools package [PT] for Mathematica. This package provides a convenient and robust way of working with MPL symbols, especially at high weight and/or height depth where the symbols become too large for calculations by hand. This package will be used for most of the calculations in the remainder of this thesis.

3.3.1 Goncharov's $\otimes^m$-invariant

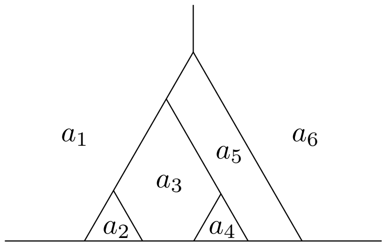
Goncharov's $\otimes^m$-invariant is defined by associating certain combinations of decorated binary trees to the MPL $I_{s_1,\ldots,s_k}(x_1,\ldots,x_k)$. The following is a synthesis of Goncharov's original description [Section 4 in Gon05], and Rhodes's very clear exposition [Section 1.2 in Rho12].

A binary tree is a rooted trivalent tree, embedded in the upper half-plane. View the tree as growing downwards towards the real line; the root extends up to ∞, and the remaining external vertices extend down to the real line. If the binary tree has $k+2$ external vertices, the $k+1$ vertices extending down to the real line will split the real line into $k+2$ intervals. These intervals can then be labelled in increasing order by elements of some list of decorations $R = [a_1, \ldots, a_{k+2}]$.

Example 3.3.1. For example the following is a binary tree with 6 external vertices, decorated with the labels $R = [a_1, \ldots, a_6]$.

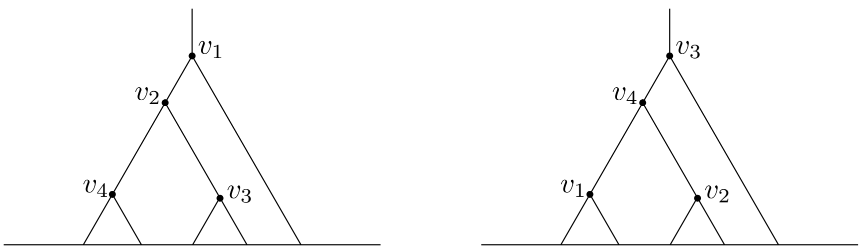


The decoration on a particular interval J can be pushed into the region of $\mathbb{H}$ which has J as part of its boundary, to get a labelling of the regions, viz:



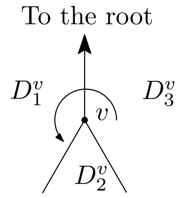
Given a such a binary tree T with $k+2$ external edges, there is a canonical partial ordering on the internal vertices of T defined by the distance from the root. We set $u \prec v$ iff there is a path from the root through u and v, and on this path u is closer to the root than v. A total ordering $v_1 < \cdots < v_k$ on the internal vertices of T, is said to be *compatible* with $\prec$ if $v_i \prec v_j$ implies $i < j$.

Example 3.3.2. Consider the two total orderings below. The left hand one is compatible with $\prec$, because any path down from the root to the real line encounters the vertices in the correct order. We either go $v_1 v_2 v_4$, or $v_1 v_2 v_3$, both of which are good. However in the right hand one, following the path $v_3 v_4 v_1$ leads to $v_4 \prec v_1$, yet $4 \not< 1$. So the right hand total order is not compatible with $\prec$.



Since the binary tree T is trivalent, every internal vertex v is on the boundary of three distinct regions D_1^v, D_2^v, D_3^v of $\mathbb{H}$. The positive (anticlockwise) orientation of the upper half-plane fixes a cyclic ordering

$D_1 \to D_2 \to D_3 \to D_1$ on these regions. From the vertex v only one edge leads to the root of T, so this allows us to canonically fix the ordering by imposing that the first region lies directly anticlockwise of the edge leading to the root.



Let $a_{D_i^v}$ be the label attached to region D_i^v in the tree T. We then attach to the vertex v the following rational function g_v^T of the labels $a_{D_i^v}$.

$$g_v^T := \begin{cases} \frac{a_{D_3^v} - a_{D_2^v}}{a_{D_1^v} - a_{D_2^v}} & \text{if all } a_{D_i^v} \text{ are distinct} \\ \frac{1}{a_{D_1^v} - a_{D_2^v}} & \text{if } a_{D_3^v} = a_{D_2^v}, \text{ but } a_{D_1^v} = a_{D_2^v} \\ \frac{a_{D_3^v} - a_{D_2^v}}{1} & \text{if } a_{D_1^v} = a_{D_2^v}, \text{ but } a_{D_3^v} \neq a_{D_2^v} \\ 1 & \text{if all } a_{D_i^v} \text{ are equal} \end{cases} \tag{3.3.1}$$

Remark 3.3.3. The expression for g_v^T that Rhodes gives in equation 1.2 of [Rho12] is only partially complete. If all the $a_{D_i^v}$ are distinct, or all are equal, then we have the same expression. But if only two of the labels are equal, then there are still two distinct labels around this vertex, and it is important to remember these in the calculation.

The definition of g_v^T is modelling the ϵ-regularisation of the integral

$$\lim_{\epsilon \to 0} \int_{a+\epsilon}^{c+\epsilon} \frac{\mathrm{d}t}{t-b} = \begin{cases} \log \frac{c-b}{a-b} & \text{if } a, b, c \text{ all distinct} \\ \log \frac{1}{a-b} & \text{if } b = c, \text{ but } a \neq b \\ \log \frac{c-b}{1} & \text{if } a = b, \text{ but } b \neq c \\ \log 1 & \text{if all } a, b, c \text{ are equal,} \end{cases}$$

as given in equation 5 of [Gon05].

Finally we are in a position to define the $\otimes^m$-invariant of an MPL. Consider an MPL

$$I := I_{s_1,\ldots,s_k}(x_1, \ldots, x_k) = I(0; x_1, \{0\}^{s_1-1}, \ldots, x_k, \{0\}^{s_k-1}; 1)\,.$$

Then I has weight $w = s_1 + \cdots + s_k$. Including the limits of the integral, it has $w + 2$ arguments, forming the following list.

$$[0, x_1, \underbrace{0, \ldots, 0}_{s_1-1}, x_2, \underbrace{0, \ldots, 0}_{s_2-1}, \ldots, x_k, \underbrace{0, \ldots, 0}_{s_k-1}, 1]\,.$$

Definition 3.3.4 ($\otimes^m$-invariant)**.** The $\otimes^m$*-invariant* (also called the *symbol*) attached to the MPL

$$I_{s_1,\ldots,s_k}(x_1, \ldots, x_k) = I(0; x_1, \{0\}^{s_1-1}, \ldots, x_k, \{0\}^{s_k-1}; 1)$$

of weight $w = s_1 + \cdots + s_k$ is denoted

$$\mathcal{S}(I_{s_1,\ldots,s_k}(x_1,\ldots,x_k)) \in \bigotimes_w \mathbb{Q}(x_1,\ldots,x_k)^* \,.$$

It is given by

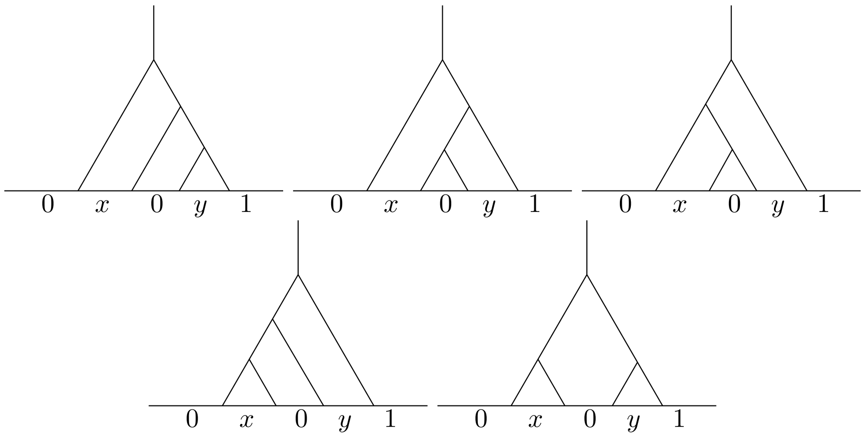
$$\mathcal{S}(I_{s_1,\ldots,s_k}(x_1,\ldots,x_k)) \coloneqq \sum_T \sum_{\{\, v_1,\ldots,v_w \,\}} g^T_{v_1} \otimes \cdots \otimes g^T_{v_w} \,,$$

where the sum over T runs over all binary trees with $w+2$ external, and decorated with the ordered labels

$$[0, x_1, \underbrace{0,\ldots,0}_{s_1-1}, x_2, \underbrace{0,\ldots,0}_{s_2-1}, \ldots, x_k, \underbrace{0,\ldots,0}_{s_k-1}, 1] \,.$$

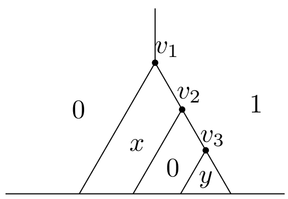
The sum over $\{\, v_1, \ldots, v_k \,\}$ runs over all total orders of the internal vertices of T which are compatible with the partial ordering $\prec$.

Example 3.3.5. We can apply the above definition to find the symbol of $I_{1,2}(x,y)$. We list the binary trees with $3+2=5$ external edges, labelled with $[0,x,y,0,1]$, as follows. There are $5 = C_3$ such trees, where $C_n = \frac{1}{2n+1}\binom{2n}{n}$ is the n-th Catalan number.



On each of the first 4 trees above, there is exactly one compatible total order, because there exists a path from the root which contains all 3 vertices of the tree. The fifth tree has two compatible total orders - the lower two vertices can be labelled v_2 and v_3 in either order.

Consider in detail the first tree, with the (unique) compatible total order of vertices, and how the decorations label the regions. We obtain

$T_1 =$ 

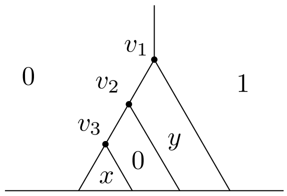
We compute that

$$g^{T_1}_{v_1} = \frac{1-x}{-x} \quad g^{T_1}_{v_2} = \frac{1}{x} \quad g^{T_1}_{v_3} = \frac{1-y}{-y} \,,$$

to obtain the following as one term in $\mathcal{S}(I_{2,1}(x,y))$

$$\{\, T_1, \{\, v_1, v_2, v_3 \,\}\,\} \rightsquigarrow \left(\frac{1-x}{-x}\right) \otimes \left(\frac{1}{x}\right) \otimes \left(\frac{1-y}{-y}\right) .$$

It turns out that the fourth and fifth trees contribute 0 to $\mathcal{S}(I_{2,1}(x,y))$ for the following reason. With the following total order

$T_4 =$ 

we have that

$$g_{v_3}^{T_4} = \frac{0-x}{0-x} = 1 .$$

But $1 \in \mathbb{Q}(x,y)^*$ is the identity element, so a term like $1 \otimes \alpha \otimes \beta$, where one tensor is 1, vanishes for the 'standard reason'. Namely

$$1 \otimes \alpha \otimes \beta + 1 \otimes \alpha \otimes \beta = (1^2) \otimes \alpha \otimes \beta = 1 \otimes \alpha \otimes \beta ,$$

then we subtract $1 \otimes \alpha \otimes \beta$ from both sides. So the fourth tree contributes 0. The fifth tree contributes 0 for the same reason.

Altogether we obtain the following result for $\mathcal{S}(I_{2,1}(x,y))$; the order of the terms matches the orders of the (non-zero) trees.

$$\begin{aligned} \mathcal{S}(I_{2,1}(x,y)) = & \left(\frac{1-x}{-x}\right) \otimes \left(\frac{1}{x}\right) \otimes \left(\frac{1-y}{-y}\right) + \\ & + \left(\frac{1-x}{-x}\right) \otimes \left(\frac{1-y}{x-y}\right) \otimes \left(\frac{y}{x}\right) + \\ & + \left(\frac{1-y}{-y}\right) \otimes \left(\frac{y-x}{-x}\right) \otimes \left(\frac{y}{x}\right) \end{aligned} \tag{3.3.2}$$

Remark 3.3.6. In any computations involving the symbol, we should always bear in mind that the following equality holds

$$\alpha \otimes \beta \otimes \gamma = \alpha \otimes (-\beta) \otimes \gamma . \tag{3.3.3}$$

This equality comes from the following calculation

$$\begin{aligned} 2 \cdot (\alpha \otimes \beta \otimes \gamma) &= \alpha \otimes \beta^2 \otimes \gamma \\ &= \alpha \otimes (-\beta)^2 \otimes \gamma \\ &= 2 \cdot (\alpha \otimes (-\beta) \otimes \gamma) . \end{aligned} \tag{3.3.4}$$

Since symbols are elements of some $\mathbb{Q}$-algebra $\bigotimes_w \mathbb{Q}(x_1, \ldots, x_k)^*$, we can divide both sides of Equation 3.3.4 by 2, and obtain Equation 3.3.3.

Consequently, the symbol of $I_{2,1}(x,y)$ can be simplified to the following

$$\begin{aligned}\mathcal{S}(I_{2,1}(x,y)) = \left(\frac{1-x}{x}\right) \otimes \left(\frac{1}{x}\right) \otimes \left(\frac{1-y}{y}\right) + \\ + \left(\frac{1-x}{x}\right) \otimes \left(\frac{1-y}{x-y}\right) \otimes \left(\frac{y}{x}\right) + \\ + \left(\frac{1-y}{y}\right) \otimes \left(\frac{y-x}{x}\right) \otimes \left(\frac{y}{x}\right) .\end{aligned}$$

3.3.2 The iterated coproduct definition

In [Gon05], Goncharov also identifies the $\otimes^m$-invariant as a maximally iterated version of his coproduct on the motivic iterated integrals from Section 1.2.1. Given a positvely graded Hopf algebra $\mathcal{A}_\bullet$, there is a canonical map

$$\Delta^{[m]} \colon \mathcal{A}_m \to \bigotimes_m \mathcal{A}_1 \, ,$$

which can be defined as the following composition

$$\mathcal{A}_m \xrightarrow{\Delta} \mathcal{A}_{m-1} \otimes \mathcal{A}_1 \xrightarrow{\Delta \otimes \mathrm{id}} \mathcal{A}_{m-2} \otimes \mathcal{A}_1 \otimes \mathcal{A}_1 \xrightarrow{\Delta \otimes \mathrm{id} \otimes \mathrm{id}} \cdots \xrightarrow{\Delta \otimes \mathrm{id}^{\otimes (m-1)}} \bigotimes_m \mathcal{A}_1 \, .$$

Then proposition 4.5 in [Gon05] claims the following equality is provable by induction on n.

Proposition 3.3.7 (Goncharov, proposition 4.5 in [Gon05])**.** *The symbol $\mathcal{S}$ arises from maximally iterating the coproduct Δ of iterated integrals*

$$\mathcal{S}(I(x_0; x_1, \ldots, x_n; x_{n+1})) \equiv \Delta^{[n]} I^{\mathcal{M}}(x_0; x_1, \ldots, x_n; x_{n+1}) \, ,$$

after making the identification

$$I^{\mathcal{M}}(a; b; c) = \log^{\mathcal{M}} \left(\frac{b-c}{b-a}\right) \leftrightsquigarrow \frac{b-c}{b-a} \, , \tag{3.3.5}$$

and performing any required regularisation.

Example 3.3.8. We can apply this iterated coproduct construction to $I_{2,1}(x,y)$, to give an alternative calculation of the symbol.

The first step is to compute the coproduct of $I_{2,1}(x,y) = I(0; x, 0, y; 1)$, and to take the $(2,1)$-degree component. For notational ease, we drop the $\mathcal{M}$ from the notation. Using Theorem 1.2.1, we compute the coproduct to be the following. Some simplifications using $I(0; a; 0) = 0$ and $I(0; 1) = 1$ are possible.

$$\begin{aligned}\Delta I(0; x, 0, y; 1) = 1 \otimes I(0; x, 0, y; 1) + \\ + I(0; x; 1) \otimes I(0; x) I(x; 0, y; 1) + I(0; 0; 1) \otimes I(0; x; 0) I(0; y; 1) + \\ + I(0; y; 1) \otimes I(0; x, 0; y) I(y; 1) + \\ + I(0; x, 0; 1) \otimes I(0; x) I(x; 0) I(0; y; 1) + I(0; x, y; 1) \otimes I(0; x) I(x; 0; y) I(y; 1) + \\ + I(0; 0, y, 1) \otimes I(0; x; 0) I(x; y) I(y; 1) + \\ I(0; x, 0, y; 1) \otimes 1\end{aligned}$$

$$\begin{aligned}&= 1 \otimes I(0; x, 0, y; 1) + I(0; x, 0, y; 1) \otimes 1 + \\ &+ I(0; x; 1) \otimes I(x; 0, y; 1) + I(0; y; 1) \otimes I(0; x, 0; y) + \\ &+ I(0; x, 0; 1) \otimes I(0; y; 1) + I(0; x, y; 1) \otimes I(x; 0; y) \,.\end{aligned}$$

So the $(2,1)$-degree component of Δ is given by

$$\Delta_{2,1} I(0; x, 0, y; 1) = I(0; x, 0; 1) \otimes I(0; y; 1) + I(0; x, y; 1) \otimes I(x; 0; y) \,.$$

Now iterate this: compute the $(1,1)$-degree component of $\Delta I(0; x, 0; 1)$ and of $\Delta I(0; x, y; 1)$. We obtain

$$\begin{aligned}&\Delta_{1,1} I(0; x, 0; 1) = I(0; x; 1) \otimes I(x; 0, 1) \\ &\Delta_{1,1} I(0; x, y; 1) = I(0; x; 1) \otimes I(x; y; 1) + I(0; y; 1) \otimes I(0; x; y) \,.\end{aligned}$$

Putting these together gives

$$\begin{aligned}\Delta^{[3]} I(0; x, 0, y; 1) = {} & I(0; x; 1) \otimes I(x; 0; 1) \otimes I(0; y; 1) + \\ & + I(0; x; 1) \otimes I(x; y; 1) \otimes I(x; 0; y) + I(0; y; 1) \otimes I(0; x; y) \otimes I(x; 0; y) \,.\end{aligned}$$

Upon using the identification from Equation 3.3.5, we obtain the symbol for $I_{2,1}(x, y)$ that we computed in Equation 3.3.2.

It has already been mentioned that the symbol is a powerful tool for finding identities and functional equations on MPL's. It does this by translating analytic problems into algebraic questions that are easier to handle. However, the symbol only captures the 'top-slice' of identities, and cannot detect anything about constant $\times$ lower weight. Since the symbol can be made to arise from the coproduct on iterated integrals, the coproduct is a good place to remedy this shortcoming. We will see this in action in Chapter 6.

3.3.3 Total differential of iterated integrals

Seeing how the differential structure of multiple polylogarithms and iterated integrals is reflected in the symbol helps us understand how we should think about and interpret the symbol. This leads to a way of directly reading the symbol from a (very particular) way of writing an iterated integral.

From Theorem 2.1 in [Gon01], we have the following computation of the total derivative of an iterated integral.

Theorem 3.3.9 (Goncharov, Theorem 2.1 in [Gon01])**.**

$$\mathrm{d} I(x_0; x_1, \ldots, x_m; x_{m+1}) = \sum_{i=1}^{m} I(x_0; x_1, \ldots, \widehat{x_i}, \ldots, x_m; x_{m+1}) \, \mathrm{d} \log \left(\frac{x_{i+1} - x_i}{x_{i-1} - x_0} \right) \,.$$

By repeatedly computing the total derivative, we 'peel off' a layer of differential forms from an iterated integral. These differential forms, written as total derivatives, give a factor of the symbol.

Starting with $I_{2,1}(x,y)$ we compute

$$\begin{aligned}\mathrm{d}I_{2,1}(x,y) =&\ \mathrm{d}I(0;x,0,y;1)\\ &= I(0;0,y;1)\,\mathrm{d}\log\left(\frac{0-x}{0-x}\right) + I(0;x,y;1)\,\mathrm{d}\log\left(\frac{0-y}{1-x}\right) + I(0;x,0;1)\,\mathrm{d}\log\left(\frac{y-1}{y-0}\right)\\ &= I(0;x,y;1)\,\mathrm{d}\log\left(\frac{-y}{1-x}\right) + I(0;x,0;1)\,\mathrm{d}\log\left(\frac{y-1}{y}\right)\,.\end{aligned}$$

So, in some sense, we have

$$I_{2,1}(x,y) = \int I(0;x,y;1)\,\mathrm{d}\log\left(\frac{0-y}{1-x}\right) + I(0;x,0;1)\,\mathrm{d}\log\left(\frac{y-1}{y-0}\right)\,.$$

Now iterate this; find $\mathrm{d}I(0;0,y;1)$ and 'peel off' a second layer of differential forms. Do this for each iterated integral appearing above.

$$\begin{aligned}\mathrm{d}I(0;x,y;1) &= I(0;y;1)\,\mathrm{d}\log\left(\frac{x-y}{x}\right) + I(0;x;1)\,\mathrm{d}\log\left(\frac{y-1}{y-x}\right)\\ \mathrm{d}I(0;x,0;1) &= I(0;x;1)\,\mathrm{d}\log\left(\frac{1}{x}\right)\,.\end{aligned}$$

And of course

$$\mathrm{d}I(a;b;c) = \mathrm{d}\log\left(\frac{b-c}{b-a}\right)\,.$$

So we can write

$$\begin{aligned}I_{2,1}(x,y) = \int &\mathrm{d}\log\left(\frac{y-1}{y}\right)\circ\mathrm{d}\log\left(\frac{x-y}{x}\right)\circ\mathrm{d}\log\left(\frac{y}{x}\right) +\\ &+ \mathrm{d}\log\left(\frac{x-1}{x}\right)\circ\mathrm{d}\log\left(\frac{y-1}{y-x}\right)\circ\mathrm{d}\log\left(\frac{y}{x}\right) +\\ &+ \mathrm{d}\log\left(\frac{x-1}{x}\right)\circ\mathrm{d}\log\left(\frac{1}{x}\right)\circ\mathrm{d}\log\left(\frac{y-1}{y}\right)\,.\end{aligned} \tag{3.3.6}$$

For an iterated integral written in the form

$$F = \int \mathrm{d}\log(f_1)\circ\cdots\circ\mathrm{d}\log(f_n)\,,$$

we read off its symbol as

$$\mathcal{S}(F) = f_1\otimes\cdots\otimes f_n\,.$$

From Equation 3.3.6, this means we get

$$\begin{aligned}\mathcal{S}(I_{2,1}(x,y)) = &\left(\frac{y-1}{y}\right)\otimes\left(\frac{x-y}{x}\right)\otimes\left(\frac{y}{x}\right) +\\ &+\left(\frac{x-1}{x}\right)\otimes\left(\frac{y-1}{y-x}\right)\otimes\left(\frac{y}{x}\right) +\\ &+\left(\frac{x-1}{x}\right)\otimes\left(\frac{1}{x}\right)\otimes\left(\frac{y-1}{y}\right)\,,\end{aligned}$$

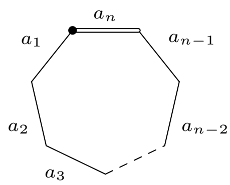
in complete agreement with the original calculation in Equation 3.3.2, up to ±1 in each tensor factor (Remark 3.3.6) and some rearrangement.

We see here how closely related the symbol is to the derivative of an iterated integral. Knowing this correspondence, it is not surprising that the symbol will capture functional equations and relations between MPL's. Requiring the symbol of a combination to be 0 will amount to forcing the derivative of this combination to be 0, so that it evaluates to a constant and gives a relation, modulo constant $\times$ lower weight terms.

3.3.4 Polygon dissections and Rhodes's hook-arrow trees

Gangl, Goncharov and Levine [GGL09] define an algebra of R-decorated polygons (R-deco for short). They then associate one of these polygons to an MPL, in such a way so that the symbol can be calculated from the combinatorics of these polygons (see as well [DGR12]). Rhodes provides a more detailed overview of this construction in Section 1.3 of [Rho12].

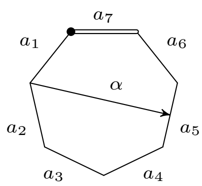
Polygons: An R-deco polygon $P(a_1, \ldots, a_n)$ is a polygon, with a specified first vertex (marked with a circle), and a final side (drawn double) giving a choice of orientation. The sides of the polygon are labelled, from first to last, by elements of the list $R = [a_1, \ldots, a_n]$, as follows.



Although not made explicit, the vertices gain an ordering $v_1, \ldots, v_n$ due to the polygon's orientation, and choice of first vertex.

The polygon algebra $\mathcal{P}^\bullet_\bullet(R)$ is generated as a vector space by wedge products of R-deco polygons. The lower grading counts the number of non-root edges in all factors of this wedge product. The upper grading counts the number of factors in the wedge product.

Arrows: The algebraic and combinatorial structure comes from arrows dissecting the polygon. By an arrow, we mean an arrow from a vertex, to a non-adjacent side. Here is an arrow α joining v_2 (the second vertex) to the side a_5.



An arrow from vertex v_i to side a_j is said to be *backwards* if $j < i$. Otherwise the arrow is *forwards.*

Dissections: These arrows let us *dissect* polygons. Given a polygon $P = P(a_1, \ldots, a_n)$, and an arrow from vertex v_i to side a_j, the polygon is dissected into two polygons

$$P_1 = (a_1, \ldots, a_{i-1}, a_j, \ldots, a_n) \quad \text{and} \quad P_2 = P(a_i, \ldots, a_j)$$

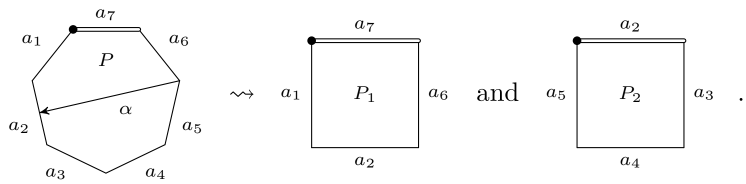
if α is a forwards arrow. Otherwise the polygon is dissected into

$$P_1 = (a_1, \ldots, a_h, a_i, \ldots, a_n) \quad \text{and} \quad P_2 = P(a_{i-1}, \ldots, a_h)$$

if α is a backwards arrow. One should think of collapsing the arrow α to pinch the polygon into two pieces – α points to the new last side, and first vertex. With this dissection, the sign of the arrow α is defined by

$$\operatorname{sgn}(\alpha) := \begin{cases} (-1)^{\#\text{non-root edges in } P_2} & \text{if } \alpha \text{ backwards} \\ 1 & \text{otherwise} \end{cases}$$

Example 3.3.10. This arrow dissects the R-deco polygon P into P_1 and P_2 as follows.

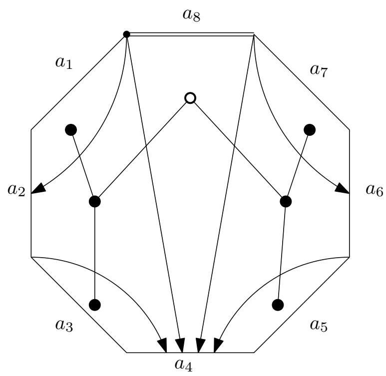


Since P_2 has three non-root edges, and the arrow α is backwards, we get that $\operatorname{sgn}(\alpha) = (-1)^3 = -1$.

Maximal dissections and the dual tree: A *maximal dissection* ρ of a polygon P is a set of $n-2$ distinct, non-crossing, dissecting arrows. The overall sign $\operatorname{sgn}(\rho)$ of the maximal dissection is $\operatorname{sgn}(\rho) = (-1)^{\#\text{backwards arrows}}$. This dissects the polygon into $n-1$ regions, which can be viewed as 2-gons.

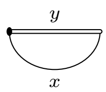
We can also consider the dual tree of this dissection. Make a point at the centre of each of the $n-1$ regions. Join two of these points with an edge if and only if the regions are share a boundary. This produces a tree graph. The first vertex and last side of the polygon P canonically defines a root vertex for the tree: the root vertex lies in the the region which contains the first vertex and (part of the) last side of P.

Example 3.3.11. The following shows a maximal dissection of the polygon $P = P(a_1, a_2, \ldots, a_8)$, along with the dual tree. The root vertex of the dual tree is marked as a hollow circle.



Now that rooted trees have appeared in the picture, we can define a partial ordering $\prec$ on the vertices of the tree according to their distance from the root. This gives a partial ordering on the regions, and hence on the 2-gons in the maximal dissection. The definition is exactly as in Section 3.3.1 for Goncharov's trivalent rooted binary trees. A total ordering on the vertices of the dual tree is said to be *compatible* with the partial ordering if $v_i \prec v_j$ implies $i < j$.

Symbol from polygons: Define the map μ on 2-gons as follows



$$\mu\left(\text{2-gon with edges } y, x\right) \coloneqq \begin{cases} 1 - \frac{y}{x} & \text{if } x, y, 0 \text{ are distinct} \\ y & \text{if } y \neq 0, \text{ but } x = 0 \\ \frac{1}{y} & \text{if } x = y, \text{ and } y \neq 0 \\ 1 & \text{otherwise.} \end{cases}$$

This map is very similar to the map $g_{v_1}^T$ from Equation 3.3.1.

We are finally in a position to define the symbol using this framework.

Definition 3.3.12 (Symbol)**.** Given an MPL $I_{s_1,\ldots,s_k}(x_1,\ldots,x_k) = I(0; x_1, \{0\}^{s_1-1}, \ldots, x_k, \{0\}^{s_k-1}; 1)$ of weight $n = s_1 + \cdots + s_k$, we attach to this the $(n+1)$-sided polygon

$$P = P(x_1, \{0\}^{s_1-1}, \ldots, x_k, \{0\}^{s_k-1}, 1))\,.$$

Then

$$\mathcal{S}(I_{s_1,\ldots,s_k}(x_1,\ldots,x_k)) \coloneqq \sum_{\rho} \operatorname{sgn}(\rho) \sum_{\{\,P_1,\ldots,P_n\,\}} \mu(P_1) \otimes \cdots \otimes \mu(P_n)\,,$$

where the first summation runs over all maximal dissections ρ of P. And the second summation runs over all compatible total orders $P_1, \ldots, P_n$ of the 2-gons.

The work in [GGL09] establishes a correspondence between the algebra of R-deco polygons and Hopf algebra of iterated integrals, meaning the construction in Definition 3.3.12 is well-defined. Specifically Proposition 8.1 in [GGL09] establishes an isomorphism from the graded Lie coalgebra $\mathcal{I}_{>0}(R)/\mathcal{I}_{>0}(R)^2$ of indecomposable iterated integrals over R to $(V_\bullet^{\mathrm{pg}}(R), \partial)$, the graded Lie coalgebra of R-deco polygons. Theorem 8.2 establishes a map of coalgebras $\langle \mathrm{B}(\pi) | \pi \in \mathcal{P}_\bullet^\bullet(R)\rangle \to \mathcal{I}_{>0}(R)^2$, comparing in detail the coproducts in each case. (Here $\mathrm{B}(\pi)$ is some element in the *bar construction* $\mathrm{B}(\mathcal{P}^\bullet_\bullet)$ that is associated to the polygon π, as in Definition 6.9 of [GGL09].) Moreover, in Chapter 3 of [Rho12], Rhodes proves explicitly that the symbol given by the polygon framework, and the $\otimes^m$ invariant given by the binary tree framework are indeed bijective.

Duhr has implemented this polygon dissection method of computing the symbol as the PolylogTools [PT] package for Mathematica. This package provides a robust and convenient way of working with MPL symbols at high weight, or high depth, which would otherwise be too cumbersome for hand calculations. The majority of calculations in this thesis have been completed using this package.

Hook-arrow trees: In Chapter 2 of [Rho12], Rhodes introduces the notation of Hook-arrow trees to solve the problem of how to represent and work with the 'visual' requirements of polygon dissections on a computer. Rhodes defines a hook-arrow tree as follows.

Definition 3.3.13 (Rhodes, Definition 2.4 in [Rho12])**.** A hook-arrow tree is a rooted spanning tree on a set of vertices in a linear order $[v_1, \ldots, v_n]$, which is not interlaced and has root v_n. The edges are directed towards v_n.

Here the vertices are meant to correspond to edges of an R-deco polygon. The term 'interlaced' means there is no choice of four vertices $v_1 < v_2 < v_3 < v_4$ such that the edges (v_1, v_3) and (v_2, v_4) are both contained in the graph. This captures the notion that edges of the spanning tree do not cross.

In Section 2.3 of [Rho12], Rhodes shows how to obtain terms in the symbol directly from these hook-arrow trees. In Chapter 4 of [Rho12], Rhode argues that the hook-arrow tree construction provides a more efficient method of computing the symbol of an MPL of given depth since one can isolate which terms will have non-zero coefficients from the start, rather than having to compute with every possible binary tree or every possible maximal dissection and see which terms happen to vanish.

Rhodes uses this to compute the symbol of $I_{a,b}(x,y)$ and $I_{a,b,c}(x,y,z)$ for arbitrary a,b,c. We will make use of the depth 2 calculation in Chapter 6 to explicitly prove an identity about $I_{a,b}(x,y) + (-1)^{a+b} I_{a,b}(\frac{1}{x}, \frac{1}{y})$ on the level of the symbol.

3.4 The symbol modulo ⧢, and modulo δ

From Section 3.2.3.2, we know that the object $-(1-x) \wedge x \otimes x^{\otimes n-2}$ attached to the polylogarithm $\mathscr{L}_n(x)$ captures the pure functional equations of $\mathscr{L}_n(x)$. Another way to view this is as the functional equations of $\mathrm{Li}_n(x)$, modulo product terms. If we compute the symbol of $\mathrm{Li}_n(x)$, we find

$$\mathcal{S}(\mathrm{Li}_n(x)) = -(1-x) \otimes x \otimes x^{\otimes n-2} .$$

So how do we go from $-(1-x) \otimes x \otimes x^{\otimes n-2}$ to $-(1-x) \wedge x \otimes x^{\otimes n-2}$ and find identities which hold modulo products? And more coarsely, can we isolate things like the pure polylogarithm components of a symbol? Or only the depth 2 contribution?

3.4.1 The symbol modulo ⧢

If we have two MPL's I_1 and I_2, with corresponding symbols $a_1 \otimes \cdots \otimes a_n$ and $b_1 \otimes \cdots \otimes b_m$, then the symbol of the product $I_1 I_2$ is given by the shuffle product of the respective symbols

$$\mathcal{S}(I_1 I_2) = \mathcal{S}(I_1) ⧢ \mathcal{S}(I_2) = a_1 \otimes \cdots \otimes a_n ⧢ b_1 \otimes \cdots \otimes b_m \,.$$

We want to introduce some operator which kills all shuffle products, leaving only the symbol modulo products. This is done in Section 5.4 of [DGR12], via the following projection operator.

Definition 3.4.1. Define a linear operator Π_w acting on elementary tensors of lengths $w \geq 1$ by $\Pi_1 = \mathrm{id}$, and for $w \geq 2$

$$\Pi_w(a_1 \otimes \cdots \otimes a_w) \coloneqq \frac{w-1}{w} \left(\Pi_{w-1}(a_1 \otimes \cdots a_{w-1}) \otimes a_w - \Pi_{w-1}(a_2 \otimes \cdots a_w) \otimes a_1 \right) \,.$$

Remark 3.4.2. The reason for the normalisation in defining Π_w is to ensure Π_w is idempotent. One might instead prefer to take the following normalisation

$$\rho_w \coloneqq w \Pi_w \,,$$

and lose the idempotency. As remarked in [DGR12], this family of operators ρ_w is already established in the shuffle algebra literature.

Proposition 1 in [DGR12] establishes the following property of Π_w, following from the same property already known for ρ_w.

Proposition 3.4.3 (Proposition 1 in [DGR12])**.** *The kernel of* Π_w *is the ideal generated by all shuffle products. That is, for any tensor* ξ*, we have*

$$\Pi_w(\xi) = 0$$

if and only if ξ *can be written as a linear combination of shuffle products.*

Example 3.4.4. By applying ρ_w, we can recover the $-(1-x) \wedge x \otimes x^{\otimes n-2}$ object corresponding to $\mathrm{Li}_n(x)$ from the symbol of $\mathrm{Li}_n(x)$.

We know that $\mathcal{S}(\mathrm{Li}_n(x)) = -(1-x) \otimes x \otimes x^{n-2}$. Computing $\rho_n(\mathcal{S}(\mathrm{Li}_n(x)))$ gives

$$\begin{aligned} \rho_n(\mathcal{S}(\mathrm{Li}_n(x))) &= \rho_n(-(1-x) \otimes x \otimes x^{n-2}) \\ &= -\rho_{n-1}((1-x) \otimes x \otimes x^{n-3}) \otimes x + \rho_{n-1}(x \otimes x^{n-2}) \otimes (1-x) \,. \end{aligned}$$

Since clearly $x \otimes \cdots \otimes x = x^{\otimes n} = \frac{1}{n!} x^{⧢ n}$ is a shuffle product, it vanishes under ρ_n, leaving

$$= \rho_{n-1}(-(1-x) \otimes x \otimes x^{\otimes n-3}) \otimes x \,.$$

Checking the base case

$$\rho(-(1-x) \otimes x) = \rho(-(1-x)) \otimes x - \rho(-(x)) \otimes (1-x)$$

$$= -(1-x) \otimes x + x \otimes (1-x)$$
$$= -(1-x) \wedge x \,,$$

establishes by induction that

$$\mathcal{S}(\mathrm{Li}_n(x)) = -(1-x) \otimes x \otimes x^{\otimes n-2} \overset{\rho_n}{\longmapsto} -(1-x) \wedge x \otimes x^{\otimes n-2}$$

In the PolylogTools package [PT], this family Π_w of operators is implemented using the command `sh`. For this reason, and since the the result of Π_w is to kill *sh*uffle products ⧢, we will refer to this as working modulo ⧢, or working modulo products.

Notation 3.4.5. In calculations involving the symbol, we write $\mathcal{S}_1 \overset{⧢}{=} \mathcal{S}_2$ to denote two symbols which are equal modulo products. That is $\rho(\mathcal{S}_1) = \rho(\mathcal{S}_2)$. (See Appendix A.)

By abuse of notation, we may also write $I \overset{⧢}{=} \mathcal{S}_1$ to mean that the iterated integral I has symbol $\mathcal{S}_1$ modulo products.

It will be convenient to write $\{x\}_n \coloneqq -(1-x) \wedge x \otimes x^{\otimes n-2}$, to reaffirm the connection of the symbol with the the Bloch groups from earlier. So $\mathcal{S}(\mathrm{Li}_n(x)) \overset{⧢}{=} \{x\}_n$.

In this notation, we have the following

Proposition 3.4.6 (Li_n inversion)**.** *On the level of the symbol, modulo products, the inversion relation says*

$$\mathcal{S}(\mathrm{Li}_n(\tfrac{1}{x})) = -(-1)^n \mathcal{S}(\mathrm{Li}_n(x)) \,.$$

So

$$\left\{\tfrac{1}{x}\right\}_n = -(-1)^n \{x\}_n \;.$$

3.4.2 The symbol modulo δ

Now we consider how to isolate and remove the depth 1 term, $\mathrm{Li}_n(x)$, from the symbol. A readable account of this, with many explicit calculations, is given in [Ver].

The origin of this process to isolate $\mathrm{Li}_n(x)$ terms lies in considering a group $\mathcal{L}_n$ describing all multiple polylogarithms of weight n, much like the Bloch group $\mathcal{B}_n$ describes the polylogarithms of weight n. (Compare with the groups $\mathcal{H}_n(E)$ that Dan defines in [Dan11], discussed in Section 5.1.2.)

Recall that $\mathcal{A}_\bullet$ is the Hopf algebra of iterated integrals from Section 1.2.1. Then we want to consider the Lie coalgebra of indecomposables

$$\mathcal{L}_\bullet \coloneqq \frac{\mathcal{A}_{>0}}{\mathcal{A}_{>0} \cdot \mathcal{A}_{>0}} \,.$$

This is the space of iterated integrals, modulo products. It inherits a Lie cobracket δ from the coproduct Δ on the Hopf algebra. This cobracket δ is defined as follows

$$\delta \coloneqq (\pi \otimes \pi) \circ (\Delta - \Delta^{\mathrm{op}}) \,,$$

where

$$\pi \colon \mathcal{A}_\bullet \to \mathcal{L}_\bullet$$

is the canonical projection map and Δ^{op} is the *opposite* coproduct. That is, if $\Delta(x) = \sum a_i \otimes b_i$, then $\Delta^{\mathrm{op}}(x) = \sum b_i \otimes a_i$. So δ defines a map

$$\delta \colon \mathcal{L}_\bullet \to \bigwedge^2 \mathcal{L}_\bullet$$

that gives $\mathcal{L}_\bullet$ the structure of a Lie coalgebra, whence $\delta^2 = 0$. Notice that for computations we can replace Δ and Δ^{op} by their respective reduced versions $\Delta' = \Delta - 1 \otimes \mathrm{id} - \mathrm{id} \otimes 1$. This is because the terms $1 \otimes x + 1 \otimes x$ will always cancel in $(\Delta - \Delta^{\mathrm{op}})(x)$.

Conjecturally, we expect exact sequences connecting $\mathcal{L}_n$, and $\mathcal{B}_n$ to arise. We can view $\mathcal{B}_n$ (weight n polylogarithms) as a subset of $\mathcal{L}_n$ (weight n *multiple* polylogarithms) in a natural way. The maps out from $\mathcal{L}_n$ are obtained from the graded components $\delta_{a,b}$ of the cobracket δ, but only the degree $(\geq 2, \geq 2)$ parts are used.

These exact sequences should give important information about weight n polylogs. At weight 4 and 5, we expect the following short exact sequences.

$$0 \to \mathcal{B}_4 \to \mathcal{L}_4 \to \bigwedge^2 \mathcal{B}_2 \to 0$$
$$0 \to \mathcal{B}_5 \to \mathcal{L}_5 \to \mathcal{B}_2 \oplus \mathcal{B}_3 \to 0 \,.$$

At weight 6, the sequence is no longer short

$$0 \to \mathcal{B}_6 \to \mathcal{L}_6 \to \mathcal{B}_3 \wedge \mathcal{B}_3 \oplus \mathcal{B}_2 \otimes \mathcal{L}_4 \to \bigwedge^3 \mathcal{B}_2 \to 0 \,.$$

Roughly one can think that the function $I_{2,2,2}(x, y, z)$, for example, genuinely has depth 3, and has a component in $\bigwedge^3 \mathcal{B}_2$.

These exact sequences mean that $\ker \bigoplus_{a,b \geq 2} \delta_{a,b}$ in $\mathcal{L}_n$ should equal (the image of) $\mathcal{B}_n$. So we can isolate and remove pure polylog terms using δ. From the conjectural existence of these exact sequences, we get the following which is a version of Zagier's polylogarithm conjecture.

Conjecture 3.4.7 (Zagier)**.** *Any expressions which vanish under $\bigoplus_{a,b \geq 2} \delta_{a,b}$ can already be written in terms of polylogarithms only.*

Indeed, we have the following easy calculation confirming that the image of $\mathcal{B}_n$ in $\mathcal{L}_n$ lands in kernel of $\bigoplus_{a,b \geq 2} \delta_{a,b}$.

Lemma 3.4.8. *Under $\bigoplus_{a,b \geq 2} \delta_{a,b}$, $\mathrm{Li}_n(x)$ maps to 0.*

Proof. $\mathrm{Li}_n(x)$ is the iterated integral $I(0; x, \{0\}^{n-1}; 1)$, up to sign and inversion of x which we can ignore.

We will talk about the coproduct Δ of $I(0; x, \{0\}^{n-1}; 1)$ using the semicircular polygon interpretation Remark 1.2.2. In order to get a degree $(\geq 2, \geq 2)$ component in Δ, we can assume $n \geq 4$.

If there is no first vertex (not including the two end points, of course), we obtain one of the trivial terms in the coproduct

$$1 \otimes I(0; x, \{0\}^{n-1}; 1)\,.$$

The first vertex of the semicircular polygon must occur at x, otherwise it would be at one of the 0's as follows

$$I(\underbrace{0; x, 0, \ldots, 0}_{\text{trivially } 0}, \ldots, 0; 1)$$

We would then obtain an integral $I(0, \ldots, 0) = 0$ in the right hand factor of the coproduct.

Now if the second vertex occurs after the second 0, it looks like follows.

$$I(0; \underbrace{x, 0, 0, \ldots, 0}_{\text{a product}}, \ldots; 1)\,.$$

So we would obtain an integral $I(x, \underbrace{0, \ldots, 0}_{k \geq 2}, 0) = \frac{1}{k!} I(x, 0, 0)^k$, which vanishes modulo products.

If the second vertex occurs at the second 0, we cannot skip any more arguments, other we would obtain $I(0; 0; 0) = 0$ or $I(0; 0; 1) \overset{\text{reg}}{=} 0$, as indicated

$$I(0; x, 0, 0, \underbrace{0, \ldots, 0}_{\text{trivially } 0}; 1) \text{ or } I(0; x, 0, 0, \underbrace{0, \ldots, 0; 1}_{\text{regularises to } 0})\,.$$

Therefore our choice of vertices is as follows,

$$I(0; \overset{\downarrow}{x}, 0, \overset{\downarrow}{0}, \overset{\downarrow}{0}, \ldots, \overset{\downarrow}{0}; 1)\,,$$

and we obtain the term

$$I(0; x, \{0\}^{n-2}; 1) \otimes \underbrace{I(0, x)}_{=1} I(x; 0; 0) \underbrace{I(0, 0) I(0, 0) \cdots I(0, 1)}_{=1}$$

in the coproduct. Since the right hand factor is weight 1, it does not contribute to $\bigoplus_{a,b \geq 2} \delta_{a,b}$.

Now it can only be the case that the second vertex occurs at the first 0. But by the same logic, we cannot skip any more arguments. Our choice of vertices is as follows,

$$I(0; \overset{\downarrow}{x}, \overset{\downarrow}{0}, \overset{\downarrow}{0}, \overset{\downarrow}{0}, \ldots, \overset{\downarrow}{0}; 1)\,,$$

and we obtain

$$I(0; x, \{0\}^{n-1}; 1) \otimes I(0, x) I(x, 0) I(0, 0) \cdots I(0, 1)\,,$$

which is nothing other than the other trivial term in the coproduct

$$I(0; x, \{0\}^{n-1}; 1) \otimes 1\,.$$

We see that there is no contribution to $\bigoplus_{a,b \geq 2} \delta_{a,b}$, so the claim holds. □

The first example in which we get a result which does not vanish under δ is for the iterated integral $I_{3,1}(x, y)$, which has a non-trivial $\delta_{2,2}$ component.

Example 3.4.9 ($I_{3,1}(x,y)$ under $\delta_{2,2}$)**.** We compute the reduced coproduct Δ' of $I_{3,1}(x,y) = I(0,x,0,0,y,1)$ to consist of the following 8 terms.

$$I(0,x,1)\otimes I(x,0,0,y,1)+I(0,y,1)\otimes I(0,x,0,0,y)+I(0,x,0,1)\otimes I(0,y,1)I(x,0,0)+$$
$$+I(0,x,0,1)\otimes I(0,0,y,1)+I(0,x,y,1)\otimes I(x,0,0,y)+I(0,x,0,0,1)\otimes I(0,y,1)+$$
$$+I(0,x,0,y,1)\otimes I(0,0,y)+I(0,x,0,y,1)\otimes I(x,0,0)$$

Of the 14 terms which should appear in the reduced coproduct, the other 6 are trivially 0 because one of the integrals involved has equal bounds $I(0,\ldots,0)=0$.

We only want to consider the $\delta_{2,2}$ component, so we throw away all but the following 3 terms.

$$I(0,x,0,1)\otimes I(0,y,1)I(x,0,0)+I(0,x,0,1)\otimes I(0,0,y,1)+I(0,x,y,1)\otimes I(x,0,0,y)\,.$$

Computing $\Delta-\Delta^{\mathrm{op}}$ has the effect of replacing $\otimes$ by $\wedge$, when going to the Lie coalgebra. We also disregard products in the Lie coalgebra, so we obtain only

$$I(0,x,0,1)\wedge I(0,0,y,1)\,.$$

The first of the 3 terms above is clearly a product in the second factor. But what happened to the third term? It also involves a product in the second factor since $I(x,0,0,y)=\frac{1}{2}I(x,0,y)^2$, using the shuffle product multiplication of iterated integrals.

We now try to convert this single remaining term back to more recognisable functions. We have $I(0,x,0,1)=-\operatorname{Li}_2(\frac{1}{x})$, and modulo products this is equivalent to $\operatorname{Li}_2(x)$ by the inversion relation. On the other hand we need to shuffle regularise $I(0,0,y,1)$. We have that

$$0=\underbrace{I(0,0,1)}_{=0}I(0,y,1)=I(0,y,0,1)+I(0,0,y,1)\,,$$

so that

$$I(0,0,y,1)=-I(0,y,0,1)=\operatorname{Li}_2(\tfrac{1}{y})\,.$$

We can therefore replace $I(0,0,y,1)$ by $-\operatorname{Li}_2(y)$ modulo products. This gives the final result that

$$\delta_{2,2}(I_{3,1}(x,y))=-\operatorname{Li}_2(x)\wedge\operatorname{Li}_2(y)\,.$$

Remark 3.4.10. The result that $\delta_{2,2}(I_{3,1}(x,y))\neq 0$ shows that it is not possible to express $I_{3,1}(x,y)$ in terms of the classical polylogarithm Li_4. So at weight 4 a genuinely new function appears. However, certain combinations of $I_{3,1}$'s can be made to vanish under $\delta_{2,2}$, which suggests that they should be expressible in terms of Li_4's. For example,

$$\delta_{2,2}(I_{3,1}(x,y)-I_{3,1}(\tfrac{1}{x},\tfrac{1}{y}))=0\,,$$

after using that $\operatorname{Li}_2(\frac{1}{x})\overset{\sqcup\!\sqcup}{=}-\operatorname{Li}_2(x)$. Gangl [Gan16] provides the following Li_4 terms for this combination

$$I_{3,1}(x,y)-I_{3,1}(\tfrac{1}{x},\tfrac{1}{y})\overset{\sqcup\!\sqcup}{=}\operatorname{Li}_4([x]-[y]+3[\tfrac{x}{y}])\,,$$

by working on the level of the symbol modulo products. Gangl [Gan16] also finds many other similar identities and functional equations between weight 4 polylogarithms, using such an approach.

How to work with δ on the symbol? For the rest of this thesis we will be working almost exclusively with the symbol of MPL's. We would therefore like a way to work with some version of δ directly on the level of symbols, rather than having to go through the coproduct, and the Lie coalgebra.

Vergu [Ver] outlines how to work with the symbol modulo δ. To compute δ of a weight n symbol, we want to project the symbol to the various different weight $(k, n-k)$ pieces and assemble these into a final result. For clarity, write $\mathcal{S}_n$ to mean the space of weight n symbols. To obtain a weight $(k, n-k)$ contribution from the symbol, we can gather the first k, and last $n-k$ tensor factors, and regard each of them as a symbol in their own right. In the Lie coalgebra $\mathcal{L}_n$, we work modulo products, so this will translate over to working with the symbol modulo products.

On symbols, we can therefore build δ up as the following composition

$$\begin{aligned}\delta = \mathcal{S}_n &\xrightarrow{\rho} \mathcal{S}_n \\ &\xrightarrow{\pi_{2,n-2} \oplus \cdots \oplus \pi_{n-2,2}} \mathcal{S}_2 \otimes \mathcal{S}_{n-2} \oplus \cdots \oplus \mathcal{S}_{n-2} \otimes \mathcal{S}_2 \\ &\xrightarrow{\rho\otimes\rho \oplus \cdots \oplus \rho\otimes\rho} \mathcal{S}_{n-2} \otimes \mathcal{S}_2 \oplus \cdots \oplus \mathcal{S}_{n-2} \otimes \mathcal{S}_2 \,,\end{aligned}$$

Here ρ is the operator which kills products from Definition 3.4.1 and Remark 3.4.2, and $\pi_{k,n-k}$ is the map which gathers the first k factors of the tensor product together, and gathers the last $n-k$ factors of the tensor product together. Informally, perhaps, we should think about identifying $\mathcal{L}_n$ with $\rho(\mathcal{S}_n)$ to aid the intuition.

The following example of the calculation of δ in the weight 4 case is found in Vergu [Ver].

Example 3.4.11. Let's see how δ acts on the symbol $a \otimes b \otimes c \otimes d$. As a first step we need to compute $a \otimes b \otimes c \otimes d$, modulo products. We get

$$\begin{aligned}a \otimes b \otimes c \otimes d \overset{\rho}{\mapsto} a \otimes b \otimes c \otimes d - b \otimes a \otimes c \otimes d - b \otimes c \otimes a \otimes d - b \otimes c \otimes d \otimes a \,+ \\ + c \otimes b \otimes a \otimes d + c \otimes b \otimes d \otimes a + c \otimes d \otimes b \otimes a - d \otimes c \otimes b \otimes a \,.\end{aligned}$$

Now gather the terms under $\pi_{2,2}$, to get

$$\begin{aligned}\xmapsto{\pi_{2,2}} (a \otimes b) \otimes (c \otimes d) - (b \otimes a) \otimes (c \otimes d) - (b \otimes c) \otimes (a \otimes d) - (b \otimes c) \otimes (d \otimes a) \,+ \\ + (c \otimes b) \otimes (a \otimes d) + (c \otimes b) \otimes (d \otimes a) + (c \otimes d) \otimes (b \otimes a) - (d \otimes c) \otimes (b \otimes a) \,.\end{aligned}$$

We can quickly check that $\rho(a \otimes b) = a \wedge b$, so applying $\rho \otimes \rho$, gives after some cancelling and regrouping

$$\begin{aligned}&\xmapsto{\rho\otimes\rho} 2(a \wedge b) \otimes (c \wedge d) - 2(c \wedge d) \otimes (a \wedge b) \\ &= 2(a \wedge b) \wedge (c \wedge d) \,.\end{aligned}$$

Therefore, on weight 4 symbols, we can compute δ as a kind of 8-fold antisymmetrisation

$$\delta(a \otimes b \otimes c \otimes d) = 2(a \wedge b) \wedge (c \wedge d)\,,$$

as was discussed in [GSVV10].

Example 3.4.12 ($I_{3,1}(x,y)$ modulo δ)**.** We can apply the above to the symbol of $I_{3,1}(x,y)$, which is

$$\begin{aligned}\mathcal{S}(I_{3,1}(x,y)) = {} & (\tfrac{1-x}{x}) \otimes (\tfrac{1}{x}) \otimes (\tfrac{1}{x}) \otimes (\tfrac{1-y}{y}) + (\tfrac{1-x}{x}) \otimes (\tfrac{1}{x}) \otimes (\tfrac{1-y}{y}) \otimes (\tfrac{1}{x}) + \\ & + (\tfrac{1-x}{x}) \otimes (\tfrac{1}{x}) \otimes (\tfrac{1-y}{y}) \otimes y + (\tfrac{1-x}{x}) \otimes (\tfrac{1-y}{x-y}) \otimes (\tfrac{y}{x}) \otimes (\tfrac{1}{x}) + \\ & + (\tfrac{1-x}{x}) \otimes (\tfrac{1-y}{x-y}) \otimes (\tfrac{y}{x}) \otimes y + (\tfrac{1-y}{y}) \otimes (\tfrac{y-x}{x}) \otimes (\tfrac{y}{x}) \otimes (\tfrac{1}{x}) + \\ & + (\tfrac{1-y}{y}) \otimes (\tfrac{y-x}{x}) \otimes (\tfrac{y}{x}) \otimes y\,.\end{aligned}$$

There are a number of simplifications to make initially. For example, we have

$$(\tfrac{1-x}{x} \wedge \tfrac{1}{x}) = -(1-x) \wedge x + x \wedge x = -(1-x) \wedge x\,,$$

which we may write as $\{x\}_2$ using the established shorthand. Similarly, we have

$$(\tfrac{y}{x}) \wedge (\tfrac{1}{x}) = -(y \wedge x) + x \wedge x = -(y \wedge x)\,.$$

Applying this to the first two terms of $\mathcal{S}(I_{3,1}(x,y))$ gives (up to a factor of 2)

$$\{x\}_2 \wedge (\tfrac{1}{x}) \wedge (\tfrac{1-y}{y}) + \{x\}_2 \wedge (\tfrac{1-y}{y}) \wedge (\tfrac{1}{x}) = 0\,.$$

Applying it to the fourth and fifth terms gives

$$((\tfrac{1-x}{x}) \wedge (\tfrac{1-y}{x-y})) \wedge (x \wedge y) - (\tfrac{1-x}{x}) \wedge (\tfrac{1-y}{x-y}) \wedge (x \wedge y) = 0\,.$$

And applying it to the sixth and seventh terms gives

$$((\tfrac{1-y}{y}) \wedge (\tfrac{y-x}{x})) \wedge (x \wedge y) - ((\tfrac{1-y}{y}) \wedge (\tfrac{y-x}{x})) \wedge (x \wedge y) = 0\,.$$

The only term which survives is the third term, and on applying δ to the third term, we obtain

$$-2\,\{x\}_2 \wedge \{y\}_2\ .$$

So under δ, we have

$$\mathcal{S}(I_{3,1}(x,y)) \overset{\delta}{\mapsto} -2\,\{x\}_2 \wedge \{y\}_2\ .$$

Notice that this agrees (upto an overall scaling) with the computation of $\delta_{2,2}(I_{3,1}(x,y))$ from Example 3.4.9, once we make the usual identification $\{x\}_2$ with the symbol of $\mathrm{Li}_2(x)$, modulo products.

Remark 3.4.13. We can see quickly that the symbol of any pure polylogarithm $\mathrm{Li}_n(x)$ vanishes under δ. The reason is simple: when $n \geq 4$, the last $n-1$ factors of $\mathcal{S}(\mathrm{Li}_n(x))$ are all x. So applying ρ to the second component of $\pi_{k,n-k}$ always yields 0, since $n-k$ ranges from 2 to $n-2$. For smaller n, there is not even enough room to split off the first and last two factors. This agrees with the result from Lemma 3.4.8.

The routine to compute the symbol modulo δ is built into Duhr's PolylogTools [PT] package as `del`. As already observed there, there appears to be some choice of scaling to be made since `del[CreateTensor[`$I_{3,1}(x,y)$`]]` returns 'essentially' $-\{x\}_2 \wedge \{y\}_2$, agreeing with Example 3.4.9. For the remainder of this thesis, any calculations involving δ will be done with Duhr's PolylogTools package to ensure consistency of results.

Notation 3.4.14. When computing with symbols $\mathcal{S}_1$ and $\mathcal{S}_2$, we shall say the symbols agree modulo δ and write $\mathcal{S}_1 \overset{\delta}{=} \mathcal{S}_2$ to mean $\delta(\mathcal{S}_1) = \delta(\mathcal{S}_2)$. (See Appendix A.)

By abuse of notation, we may also write $I \overset{\delta}{=} \mathcal{S}_1$ to mean the iterated integral I has symbol $\mathcal{S}_1$ modulo δ.

According to Zagier's conjecture, Conjecture 3.4.7, when working with the symbol modulo δ we should think that this is the symbol modulo the depth 1 terms Li_n. Given the conjectural status of this result, we will typically say that some result which vanishes modulo δ is 'morally' expressible in terms of Li_n to avoid treating this conjecture as an inviolable truth. A similar construction appears to exists to work modulo depth 2 terms, or even higher by iterating and considering some 'version' of δ, δ^2, *et cetera*. I will touch on this slightly in Remark 7.8.2, although since $\delta^2 = 0$ on $\mathcal{L}_\bullet$, it is perhaps not entirely clear how this construction should be interpreted.

3.4.2.1 Nielsen polylogarithms and the kernel of δ

Zagier's conjecture that the kernel of δ consists exactly of classical polylogarithms Li_n, Conjecture 3.4.7, usually works very well in explicit computations. That is to say, given some combination with symbol $\mathcal{S}_1$ that vanishes modulo δ, it is usually possible to generate a large enough set of 'good arguments' (through intuition, analogy with lower weight cases, or semi-exhaustive computation using packages like Danylo Radchenko's MESA [MESA]) to find Li_n terms which agree with the symbol $\mathcal{S}_1$ modulo products.

However, there is a special class of iterated integrals which appears to be something of an obstruction to this. As Brown notes [Bro], the *a priori* slightly larger class of *Nielsen polylogarithms* [Nie09], also vanishes modulo δ.

Definition 3.4.15 (Nielsen polylogarithm)**.** The Nielsen polylogarithm $S_{n,p}(x)$ is defined by the iterated integral

$$S_{n,p}(x) \coloneqq (-1)^p I(0; \{1\}^p, \{0\}^n; x) .$$

We readily compute the symbol of $S_{n,p}(x)$ to be

$$\mathcal{S}(S_{n,p}(x)) = (-1)^p (1-x)^{\otimes p} \otimes x^{\otimes n} ,$$

and observe that $S_{n-1,1}(x) = \mathrm{Li}_n(x)$ is the usual polylogarithm.

Proposition 3.4.16. *Under δ, the symbol of the Nielsen polylogarithm $S_{m,p}(x)$ of weight $n = m + p$ goes to 0.*

Proof. For weight ≤ 3, δ always vanishes because there is not enough room to compute a non-trivial result. When weight ≥ 4, we find that the first p positions agree and last m positions agree.

$$\mathcal{S}(S_{m,p}(x)) = \pm \underbrace{(1-x) \otimes \cdots \otimes (1-x)}_{p \text{ positions}} \otimes \underbrace{x \otimes \cdots \otimes x}_{m \text{ positions}}$$

The contribution for $(\rho \otimes \rho) \circ \pi_{k,n-k}$ is 0 whenever $k \leq p$ because the first ρ vanishes. Otherwise, when $k > p$, we have $n - k < n - p = m$, to the contribution for $(\rho \otimes \rho) \circ \pi_{k,n-k}$ still vanishes because the second ρ vanishes. Overall, all terms in $\delta\mathcal{S}(S_{m,p}(x))$, vanish as claimed. ☐

Remark 3.4.17. The truth of Conjecture 3.4.7 would imply that the Nielsen polylogarithms $S_{m,p}(x)$ can be expressed in terms of Li_n. Indeed, we can give the following symbol level expression for $S_{2,2}(x)$

$$\begin{aligned} S_{2,2}(x) &\overset{\mathcal{S}}{=} \mathrm{Li}_4\left([x] - [1-x] + \left[\frac{x}{x-1}\right]\right) + \\ &\quad - \mathrm{Li}_3(x)\log(1-x) - \frac{1}{6}\log(x)\log(1-x)^3 + \frac{1}{24}\log(1-x)^4 \,. \end{aligned}$$

Unfortunately, despite many extensive attempts, I have not been able to find a reduction of $S_{3,2}(x)$ to classical polylogarithms.

However, we can relate all of the different Nielsen polylogarithms in weight 5, 6 and 7 back to $S_{n-2,2}(x)$ and $\mathrm{Li}_n(x)$, as follows. Generally it appears that $S_{a,b}(x) \overset{⧢}{=} -S_{b,a}(1-x)$. Then the remaining cases are

$$\begin{aligned} S_{3,3}(x) &\overset{⧢}{=} 2\,\mathrm{Li}_6\,(1-x) + \frac{1}{2} S_{4,2}\left([x] - 3[1-x] - \left[\frac{x}{x-1}\right]\right) \\ S_{4,3}(x) &\overset{⧢}{=} \mathrm{Li}_7\left(-3[x] + 2[1-x] - 3\left[\frac{x}{x-1}\right]\right) + S_{5,2}\left([x] - [1-x] + \left[\frac{x}{x-1}\right]\right) . \end{aligned}$$

Somehow $S_{n-2,2}(x)$ and $\mathrm{Li}_n(x)$ seem to be the 'basic' functions which vanish modulo δ, in weight ≤ 7. Therefore the question of characterising $\ker\delta$ here is reduced to determining whether or not $S_{n-2,2}(x)$ can be expressed in terms of the classicl polylogarithm $\mathrm{Li}_n(x)$. Starting at weight 8 further obstructions appear, for example $S_{5,3}(x)$ does not seem to be expressible in terms of $S_{n-2,2}(x)$ and Li_n, without searching again for yet more 'good arguments'.

When studying weight ≥ 5 multiple polylogarithm functional equations in Chapter 4, and Chapter 7, we will explicitly allow Nielsen $S_{n-2,2}(x)$ terms when attempting to find the terms missing 'depth 1' terms in symbol level identities. That is to say, we shall leave resolving the question of whether Li_n is exactly the kernel of δ as a problem for future investigation. Indeed, without yet having a reduction of $S_{3,2}(x)$ to Li_5's, there are definitely times when Nielsen terms *appear* to be necessary, starting already in Section 4.2.1.3.

Remark 3.4.18. Finally, it is curious to note that modulo ⧢, we have

$$S_{n-2,2}(x) \overset{⧢}{=} I_{n-1,1}(1,x) + n\,\mathrm{Li}_n(x) \,.$$

So that the Nielsen polylogarithm $S_{n-2,2}(x)$ can be expressed via some kind of 'single-variable' depth 2 integral.

Chapter 4

Relating weight 5 MPL's

In this chapter we shall investigate the symmetries and relations between various weight 5 MPL's, following previous investigations by Gangl [Gan16] in the weight 4 case. We try to motivate this investigation by claiming that in order to understand the weight 5 polylogarithm, one really needs to understand how it fits into the broader context of weight 5 multiple polylogarithms (Section 4.1.1).

From the start, we restrict to a relatively small but potentially interesting set of arguments of the form $[\mathrm{cr}(a, b, c, d_1), \ldots, \mathrm{cr}(a, b, c, d_k)]$ ("coupled cross-ratios", Notation 4.1.1). We discuss the potential computational difficulties (memory and CPU time, Section 4.1.3.1) in finding all relations between iterated integrals with these arguments, and some of the strategies to minimise these such as the "numerical valuations" idea from Danylo Radchenko.

We start by looking for symmetries, and short functional equations, for the weight 5 depth 2 iterated integrals. We do this first for $I_{4,1}$ using 'coupled cross-ratio' arguments, modulo δ (Section 4.2.1). Then we try to lift them to identities for $I_{4,1}$ holding modulo products (Section 4.2.1.3), and even on the level of the symbol (Section 4.2.1.1, Section 4.2.1.2). We encounter an 'obstruction' in the form of Nielsen polylogarithms when trying to lift some of these identities (Section 4.2.1.3). We then repeat this process for the multiple polylogarithm $I_{3,2}$ (Section 4.2.2), and we determine how $I_{4,1}$ and $I_{3,2}$ relate (Section 4.2.2.3)

Next we will investigate identities holding between depth 3 MPL's using 'coupled cross-ratio' arguments (Section 4.3). We look for identities on $I_{3,1,1}$ modulo δ (Section 4.3.1). However, it turns out that allowing a small selection of $I_{3,2}$ terms (but not so many as to make everything trivial) drastically simplifies the structure of the relations amongst depth 3 MPL's (Section 4.3.2 onwards). We can even explicitly lift the identities for $I_{3,1,1}$ mod $I_{3,2}$ to identities modulo products (Section 4.3.2.2) Moreover, we find the curious result (Theorem 4.3.18) that any depth 3 MPL is equivalent modulo these $I_{3,2}$ terms to a sum over any other depth 3 MPL.

Finally, we indicate some results which occur at higher depths, such as a reduction of $I_{2,1,1,1}$ to $I_{3,1,1}$'s, and some short functional equations for $I_{1,1,1,1,1}$ (Section 4.4). We also suggest a larger set of arguments which might lead to 'better' identities between weight 5 MPL's Section 4.4.3).

4.1 Introduction

4.1.1 Motivation

In order to understand better the behaviour of the weight 5 polylogarithm Li_5, it becomes important to understand how it fits into the more general picture of *multiple* polylogarithms. For example, in Section 7.4 an idea of Goncharov's will let us find functional equations for Li_5 by studying the iterated integral $I_{4,1}$. The pure polylogarithms Li_n cannot be treated in isolation without losing far too much of the important structure which comes from the multiple polylogarithms. Indeed, Gangl has made a similar study of the weight 4 case [Gan16], and by understanding how certain combinations of depth 2 iterated integrals relate has been able to find a highly generic Li_4 functional equation using Goncharov's idea for weight 4. This will again be discussed in Chapter 7.

4.1.2 Notation and goal

We will initially look at symmetries of iterated integrals $I_{a_1,\ldots,a_n}(x_1,\ldots,x_n)$, where the arguments are cross-ratios. There are two main reasons for restricting to this choice of arguments. The first reason is that Gangl [Gan16] has had a great deal of success analysing such arguments in the weight 4 case. A second, deeper, reason for this choice of arguments has to do with the connection to the geometry of the moduli space $\mathfrak{M}_{0,n}$, of n marked points on $\mathbb{P}^1$, with cross-ratios providing a natural choice of coordinates on $\mathfrak{M}_{0,n}$. For further details of the connection between multiple polylogarithms and $\mathfrak{M}_{0,n}$, see Section 6 of [Bro09]. In particular, Corollary 6.17 of [Bro09], shows that every iterated integral on $\mathfrak{M}_{0,n}$ can be expressed as a sum of products of multiple polylogarithms of the form

$$\mathrm{Li}_{n_1,\ldots,n_r}\left(\frac{x_{j_1}\cdots x_\ell}{x_{j_2}\cdots x_\ell},\ldots,\frac{x_{j_{r-1}}\cdots x_\ell}{x_{j_r}\cdots x_\ell},\ldots,x_{j_r}\cdots x_\ell\right),$$

and logarithms $\log(x_1),\ldots,\log(x_\ell)$, where $x_1,\ldots,x_\ell$ are *cubical coordinates* on $\mathfrak{M}_{0,n}$, and $1\leq j_1,\ldots,j_r\leq\ell$ are any indices.

Given 4 points a,b,c,d, we will abbreviate the cross-ratio as follows

$$abcd \coloneqq \mathrm{cr}(a,b,c,d) = \frac{a-c}{a-d}\Big/\frac{b-c}{b-d}\,.$$

Then if we have an iterated integral with cross-ratio arguments $I_{n_1,\ldots,n_k}(abcd_1, abcd_2,\ldots,abcd_k)$, we will abbreviate this to

$$I_{n_1,\ldots,n_k}(abcd_1d_2\ldots d_k) \coloneqq I_{n_1,\ldots,n_k}(abcd_1, abcd_2,\ldots,abcd_k)\,.$$

For example

$$I_{3,2}(abcde) = I_{3,2}(\mathrm{cr}(a,b,c,d),\mathrm{cr}(a,b,c,e))\,.$$

This does have the effect of strongly *coupling* the variables together, and so restricts the scope for finding identities and relations. But at the same time, this gives us a tractable set of arguments to work with initially, so that the task of finding relations is not hopelessly open-ended.

Notation 4.1.1 (Coupled cross-ratio arguments)**.** We will call arguments of the form $[abcd, abce] = [\mathrm{cr}(a,b,c,d), \mathrm{cr}(a,b,c,e)]$, or more generally $[abcd_1, \ldots, abcd_k] = [\mathrm{cr}(a,b,c,d_1), \ldots, \mathrm{cr}(a,b,c,d_k)]$, *coupled cross-ratio* arguments.

From here we can expand to relations between different iterated integrals, using a similar set up with cross-ratio arguments.

We will look for symmetries and relations with varying levels of accuracy. On the coarsest level, we will look modulo δ, meaning (roughly) the identities hold modulo depth 1 terms, i.e. modulo Li_n. With persistence maybe these identities can be upgraded to identities holding modulo $⧢$, that is modulo products. In some cases it may even be possible to find identities which hold on the level of the symbol exactly.

It does not (quite) make sense to look for identities holding 'modulo δ^2' since one expects that every iterated integral at weight 5 can already be written in terms of I_5, $I_{3,2}$ and $I_{2,3}$ by eliminating the indices 1. This would mean that *every* weight 5 iterated integral vanishes 'modulo δ^2'. This is investigated in more depth in Section 5.3. However, it could be worth asking for relations which hold true modulo depth 2 integrals with our (relatively) simple choice of cross-ratio arguments.

4.1.3 Strategy for finding relations

The basic strategy for finding relations between these types of iterated integrals is to apply brute-force linear algebra. For example, to find relations for $I_{4,1}$ modulo δ, form the linear combination

$$T = \sum_{\sigma \in S_{\{\, a,b,c,d,e \,\}}} c_\sigma I_{4,1}(\sigma \cdot abcde) \,.$$

Then compute the symbol $\mathcal{S}(T)$, and reduce modulo δ. Setting this combination to 0 produces a linear system of equations for the coefficients c_σ, which can then be solved to find relations for $I_{4,1}$ modulo δ.

4.1.3.1 Dealing with 'potentially' large systems of equations

This method of brute-force computing the symbol and setting up a large system of equations works insofar as low depth, low weight integrals can be analysed like this. The main bottle-neck initially is computing the symbol of each term. Already the symbol of $I_{4,1}(abcde)$ modulo δ involves 4536 terms when fully expanded out to elementary tensors. Summing over $5! = 120$ different permutations of $abcde$ involves over half a million terms, taking up nearly 700 MB of memory. The intermediate calculations in Mathematica require 4.6 GB of memory. For a higher depth integral like $I_{3,1,1}$, the symbol for a single term of $I_{3,1,1}(abcdef)$ modulo δ has 23256 terms. Then we would sum over $6! = 720$ different terms, so the result would be approximately 30 times bigger already.

This large number of terms feeds into the next bottle-neck. The resulting system of equations is *hideously* over-determined. In the case of $I_{4,1}$ modulo δ, by setting the sum $\mathcal{S}(T) = 0$ modulo δ, we obtain 45360 equations for the $5! = 120$ variables c_σ. Even removing exact duplicates still leads to 4200 equations. But the rank of the resulting matrix is only 20, meaning 4180 of these equations are completely redundant!

Numerical valuations: From discussions with Danylo Radchenko, I learned of a better way to generate the system of equations for the c_σ. Given a symbol (modulo ⧢, modulo δ, or otherwise) $s \in \bigotimes_n \mathbb{Q}(x_1, \ldots, x_\ell)^*$ one specialises each $x_1, \ldots, x_\ell$ to some sufficiently generic tuple of rationals (or even integers), giving a map $\bigotimes_n \mathbb{Q}(x_1, \ldots, x_\ell)^* \to \bigotimes_n \mathbb{Q}^*$. In this context generic means no pairs $x_i = x_j$ are allowed, and all x_i are away from poles of factors of s.

Now choose a set of n primes $p_1, \ldots, p_n$, and compute the valuation ν_{p_i} of tensor factor i with respect to prime p_i, and take the product of the results. This gives a map $\bigotimes_n \mathbb{Q}^* \to \mathbb{Q}^*$. (Remember that we treat tensors as multiplicative rather than additive in each slot $(ab) \otimes c = a \otimes c + b \otimes c$.) On an elementary tensor $q_1 \otimes \cdots \otimes q_n \in \mathbb{Q}^{\otimes n}$, we obtain

$$q_1 \otimes \cdots \otimes q_n \mapsto \nu_{p_1}(q_1) \cdots \nu_{p_n}(q_n) \,.$$

Overall we obtain a map $N = N_{x_1, \ldots, x_\ell, p_1, \ldots, p_n} \colon \bigotimes_n \mathbb{Q}(x_1, \ldots, x_\ell)^* \to \mathbb{Q}^*$, by extending formally to symbols which are linear combinations of elementary tensors.

Applying this construction to $\mathcal{S}(T) = 0$, above, leads to

$$\sum_{\sigma \in S_{\{\, a,b,c,d,e \,\}}} c_\sigma \underbrace{N(\mathcal{S}(I_{4,1}(\sigma \cdot abcde)))}_{\in \mathbb{Q}} = 0 \,.$$

So for each choice of specialisations, and primes, we produce one equation for the c_σ. By choosing different specialisations and/or different primes, we obtain further equations for the c_σ. The linear system can therefore be built up one equation at a time until the rank stabilises, and no new equations for the c_σ arise.

Generating the system of equations this way had further advantages over the brute-force ‘compute and expand out the symbol’ approach.

Firstly, the symbol of $I_{4,1}(\sigma \cdot abcde)$ arises by plugging suitable arguments (namely, $\sigma \cdot abcd$, and $\sigma \cdot abce$) into $I_{4,1}(x, y)$. So we can compute $N(\mathcal{S}(I_{4,1}(\sigma \cdot abcde)))$ by first specialising the arguments, then using the numerical valuation coming from $I_{4,1}(x, y)$. This means we only need to compute the symbol of $I_{4,1}$ once, but can use it again and again for new choices of arguments. Moreover, the map N does not depend on the particular presentation chosen for the symbol, so we are free to use the most compact version we can.

For example, the version of the symbol produced by Goncharov’s tree definition (Section 3.3.1) is significantly shorter than than the version produced by Duhr’s PolylogTools package. Not least of which this is because Duhr’s package necessarily must reduce the symbol to elementary tensors before returning the result. Instead, I can implement my own version of Goncharov’s tree definition to compute the symbol for these calculations. I find (of course!) that it agrees with Duhr's results in every case, whilst making some of computations much more efficient.

Another advantage comes from noticing that the calculations of N for different specialisations, and for different primes, are completely independent. Therefore multiple calculations of N can be run in *parallel*, further reducing the computation time of the system of equations for c_σ.

4.1.3.2 Finding 'short' relations

Besides generating the matrix, another difficulty lies in finding 'nice' relations. Typically one wants relations with integer coefficients (or rationals with small very small denominators). Moreover, one wants relations with relatively few terms, roughly meaning short null vectors in one metric or another.

Gaussian elimination to find the nullspace of the resulting matrix will not lead to particularly nice relations. One can try to use LLL reduction to find 'better' integer basis for the nullspace. In Mathematica [MA] this can be done with the command `LatticeReduce`. Better results can be obtained by passing the matrix to GP/Pari [GP], for processing with the `matkerint` command.

These routines do not guarantee the shortest possible relations, but in practice they typically work well enough to identity very short relations. Due to the setup of the problem, any permutation of arguments *abcde* in an identity necessarily produces another identity. By finding a short null-vector, and generating further short null-vectors in the null-space, one can `LatticeReduce` several times to try to find the shortest possible relations.

4.2 Depth 2 iterated integrals

At depth 2, there are four iterated integrals to consider, namely $I_{4,1}$, $I_{3,2}$, $I_{2,3}$ and $I_{1,4}$. In some sense, $I_{4,1}$ is the simplest of these, having the shortest symbol, so it is best to start there.

4.2.1 Relations for $I_{4,1}$ modulo δ

Firstly we look for relations which hold modulo products, and depth 1 terms. That is modulo δ. We find some simple two term identities of the following form.

Identity 4.2.1. *Modulo δ, we have*

$$I_{4,1}(abc(de)) \overset{\delta}{=} I_{4,1}(abc(ed)) \tag{4.2.1a}$$

$$I_{4,1}((ab)cde) \overset{\delta}{=} -I_{4,1}((ba)cde)\,. \tag{4.2.1b}$$

Remark 4.2.2. In these identities, and any subsequent ones, the bracketing of cross-ratio arguments is only for emphasis. It is there only to help identify which variables in the cross-ratios have changed.

Converting back from cross-ratios to rational functions, by setting $a = \infty$, $b = 0$, $c = 1$, $d = x$ and $e = y$, we can write these identities as

$$I_{4,1}(x,y) \overset{\delta}{=} I_{4,1}(y,x) \tag{4.2.1a$'$}$$

$$I_{4,1}(x,y) \overset{\delta}{=} -I_{4,1}(\tfrac{1}{x},\tfrac{1}{y})\,. \tag{4.2.1b$'$}$$

We will see identities like Equation 4.2.1b′ occur for all of the depth 2 iterated integrals $I_{a,b}$. Indeed, Chapter 6 deals with providing a general proof of this result, and lifting a certain subclass of identities, those for $I_{n,1}$ to full numerically testable identities.

Potentially more interesting is the following cyclically symmetric identity

Identity 4.2.3. *Modulo δ we have*

$$\operatorname{Cyc}_{a,b,c} I_{4,1}((abc)de) = I_{4,1}((abc)de) + I_{4,1}((bca)de) + I_{4,1}((cab)de) \overset{\delta}{=} 0 \tag{4.2.2}$$

Or equivalently,

$$I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{1-x},\tfrac{1}{1-y}) + I_{4,1}(1-\tfrac{1}{x},1-\tfrac{1}{y}) \overset{\delta}{=} 0\,. \tag{4.2.2$'$}$$

The above identities hold modulo δ, which morally means modulo Li_5 terms and products. We should try to find the missing Li_5 terms in order to get identities which hold modulo $\sqcup\!\sqcup$.

4.2.1.1 Li_5 and product terms for symmetry $I_{4,1}(x,y) \overset{\delta}{=} I_{4,1}(y,x)$

Identity 4.2.4. *Modulo $\sqcup\!\sqcup$ we have*

$$I_{4,1}(abc(de)) \overset{\sqcup\!\sqcup}{=} I_{4,1}(abc(ed)))\,,$$

so Equation 4.2.1a holds modulo $\sqcup\!\sqcup$ already.

Or equivalently

$$I_{4,1}(x,y) \overset{\sqcup\!\sqcup}{=} I_{4,1}(y,x)\,.$$

A similar result is observed by Gangl in [Gan16] at weight 4, where it is stated that $I_{3,1}(x,y) \overset{\sqcup\!\sqcup}{=} -I_{3,1}(y,x)$. Both of these symmetries are instances of the following general result.

Proposition 4.2.5. *The following identity holds exactly for the iterated integrals.*

$$I_{n,1}(x,y) - (-1)^n I_{n,1}(y,x) = (-1)^n \sum_{i=1}^{n} (-1)^i I_i(x) I_{n+1-i}(y)\,. \tag{4.2.3}$$

So modulo $\sqcup\!\sqcup$, we obtain

$$I_{n,1}(x,y) \overset{\sqcup\!\sqcup}{=} (-1)^n I_{n,1}(y,x)$$

Proof. We firstly convert this to a result on differential forms, then we can use that the product of iterated integrals is just the shuffle product of the word describing the differential forms, as in the shuffle product property of Property 1.1.13. On the right hand side of Equation 4.2.3, ignoring the factor $(-1)^n$, we have

$$\sum_{i=1}^{n}(-1)^i I_i(x) I_{n+1-i}(y) = \sum_{i=1}^{n}(-1)^i I(0; x, \{0\}^{i-1} \mid 1) I(0 \mid y, \{0\}^{n-i}; 1) \, .$$

So really we want to evaluate the following combination of differential words

$$\sum_{i=1}^{n}(-1)^i (x0^{i-1}) \sqcup\!\sqcup (y0^{n-i}) \, .$$

By explicitly multiplying out and checking cases $n < 3$, we can assume $n \geq 3$ without loss of generality. Then we can separate the $i = 1$ and $i = n$ terms of the sum to obtain

$$= -x \sqcup\!\sqcup (y0^{n-1}) + (-1)^n (x0^{n-1}) \sqcup\!\sqcup y + \sum_{i=2}^{n-1}(-1)^i (x0^{i-1}) \sqcup\!\sqcup (y0^{n-i}) \, .$$

Using the recursive definition of the shuffle product, we have

$$(x0^{i-1}) \sqcup\!\sqcup (y0^{n-i}) = \big(x0^{i-2} \sqcup\!\sqcup (y0^{n-i})\big) 0 + \big((x0^{i-1}) \sqcup\!\sqcup (y0^{n-1-i})\big) 0 \, .$$

Plugging this back into the sum, we obtain

$$\begin{aligned} = -x \sqcup\!\sqcup (y0^{n-1}) + (-1)^n (x0^{n-1}) \sqcup\!\sqcup y + \sum_{i=2}^{n-1} \bigg(& (-1)^i \big(x0^{i-2} \sqcup\!\sqcup (y0^{n-i})\big) 0 + \\ & - (-1)^{i+1} \Big((x0^{i-1}) \sqcup\!\sqcup (y0^{n-(i+1)}) \Big) 0 \bigg) \, . \end{aligned}$$

But now this sum telescopes, leaving only

$$= -x \sqcup\!\sqcup (y0^{n-1}) + (-1)^n (x0^{n-1}) \sqcup\!\sqcup y + \Big((x \sqcup\!\sqcup (y0^{n-2}))0 - (-1)^n ((x0^{n-2}) \sqcup\!\sqcup y)0 \Big) \, .$$

Finally we can rearrange the recursive definition of the shuffle product to get

$$\begin{aligned} -x \sqcup\!\sqcup (y0^{n-1}) + (x \sqcup\!\sqcup (y0^{n-2}))0 &= -(\emptyset \sqcup\!\sqcup y0^{n-1})x \\ (x0^{n-1}) \sqcup\!\sqcup y - ((x0^{n-2}) \sqcup\!\sqcup y)0 &= (x0^{n-1} \sqcup\!\sqcup \emptyset)y \, . \end{aligned}$$

Plugging these into the previous shows that the right hand side is

$$= -(\emptyset \sqcup\!\sqcup (y0^{n-1}))x + ((x0^{n-1}) \sqcup\!\sqcup \emptyset)y = -(y0^{n-1}x) + (-1)^n (x0^{n-1}y)$$

Taking the iterated integral of this result shows that

$$\begin{aligned} & \sum_{i=1}^{n}(-1)^i I(0; x, \{0\}^{i-1}; 1) I(0; y, \{0\}^{n-i}; 1) = \\ & \qquad - I(0; y\{0\}^{n-1}x; 1) + (-1)^n I(0; x\{0\}^{n-1}y; 1) \, . \end{aligned}$$

Multiplying by $(-1)^n$, and using the usual shorthand notation $I_{a,b}(x, y) \leftrightarrow I(0; x\{0\}^{a-1}y\{0\}^{b-1}; 1)$, gives the desired identity. □

So in fact we can add the missing product terms to get an identity which holds on the level of the symbol. For psychological reasons, one might prefer to write this in terms of the usual polylogarithms, rather than depth 1 iterated integrals. This can be done using the equivalence

$$\mathrm{Li}_n(x) = -I_n(\tfrac{1}{x})\,.$$

Identity 4.2.6. *The following identity holds on the level of the symbol.*

$$I_{4,1}(x,y) - I_{4,1}(y,x) \overset{\mathcal{S}}{=} -\mathrm{Li}_1(\tfrac{1}{x})\,\mathrm{Li}_4(\tfrac{1}{y}) + \mathrm{Li}_2(\tfrac{1}{x})\,\mathrm{Li}_3(\tfrac{1}{y}) - \mathrm{Li}_3(\tfrac{1}{x})\,\mathrm{Li}_2(\tfrac{1}{y}) + \mathrm{Li}_4(\tfrac{1}{x})\,\mathrm{Li}_1(\tfrac{1}{y})\,.$$

More generally, the following holds on the level of the symbol.

$$I_{n,1}(x,y) - (-1)^n I_{n,1}(y,x) \overset{\mathcal{S}}{=} \sum_{i=1}^{n} (-1)^{n-i}\,\mathrm{Li}_i(\tfrac{1}{x})\,\mathrm{Li}_{n+1-i}(\tfrac{1}{y})\,.$$

4.2.1.2 Li_5 and product terms for symmetry $I_{4,1}(x,y) \overset{\delta}{=} -I_{4,1}(\frac{1}{x},\frac{1}{y})$

The identity in Equation 4.2.1b does *not* hold modulo ⧢, so we do need to find Li_5 terms which make it hold. Some brief searching with Mathematica uncovers the necessary Li_5 terms, giving the following result.

Identity 4.2.7. *The following identity holds modulo products.*

$$I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x},\tfrac{1}{y}) \overset{⧢}{=} \mathrm{Li}_5\left(-[x] - [y] - 4\left[\tfrac{x}{y}\right]\right)$$

This identity should be compared with the corresponding weight 4 identity in [Gan16], which states

$$I_{3,1}(x,y) - I_{3,1}(\tfrac{1}{x},\tfrac{1}{y}) = \mathrm{Li}_4\left([x] - [y] + 3\left[\tfrac{x}{y}\right]\right)\,.$$

With some further searching, we can find product terms which make the identity hold exactly on the level of the symbol.

Identity 4.2.8. *The following identity holds exactly on the level of the symbol.*

$$\begin{aligned} I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x},\tfrac{1}{y}) &\overset{\mathcal{S}}{=} \mathrm{Li}_5\left(-[x] - [y] - 4\left[\tfrac{x}{y}\right]\right) + \\ &+ \mathrm{Li}_4(y)\log(x) - \tfrac{1}{2!}\mathrm{Li}_3(y)\log^2(x) + \tfrac{1}{3!}\mathrm{Li}_2(y)\log^3(x) - \tfrac{1}{4!}\mathrm{Li}_1(y)\log^4(x) + \\ &+ \mathrm{Li}_4\left(\tfrac{x}{y}\right)\log\left(\tfrac{x}{y}\right) + \tfrac{1}{5!}\left(\log^5\left(\tfrac{x}{y}\right) - \log^5(x)\right) \end{aligned}$$

Again, this should be compared with the symbol level identity for $I_{3,1}(x,y) - I_{3,1}(\frac{1}{x},\frac{1}{y})$ presented in [Gan16]. Even if not exactly equivalent, these two identities overwhelmingly share the same structures. The similarities between these identities at weight 4 and weight 5 will be explored further in Chapter 6. There, a general symbol level identity which holds for any iterated integral $I_{a,b}(x,y)$ will be proven. Moreover using slices of the multiple polylogarithm coproduct, the $I_{n,1}(x,y)$ case will be lifted to a candidate numerically testable identity, like Duhr does using Gangl's weight 4 identity for $I_{3,1}(x,y)$.

4.2.1.3 Li_5 and Nielsen terms for relation $\mathrm{Cyc}_{\{a,b,c\}} I_{4,1}((abc)de) \overset{\delta}{=} 0$

The 3-term identity in Equation 4.2.2 also needs Li_5 terms to complete it to an identity which holds modulo $⧢$. But here we encounter our first surprise! At weight ≥ 5, it is only a rule of thumb that vanishing modulo δ means Li_5 terms (hence the 'morally' everywhere). As Brown notes [Bro], the class of functions which vanish modulo δ is strictly larger than Li_n in general – one also needs to introduce Nielsen polylogarithms (see Section 3.4.2.1).

In this case we find the following Li_5 and Nielsen terms.

Identity 4.2.9. *The following identity holds modulo products.*

$$\begin{aligned} I_{4,1}(x,y) + I_{4,1}(1-\tfrac{1}{x}, 1-\tfrac{1}{y}) + I_{4,1}(\tfrac{1}{1-x}, \tfrac{1}{1-y}) \overset{⧢}{=} {} & -2\,\mathrm{Li}_5(\tfrac{x}{y}) - 2\,\mathrm{Li}_5(\tfrac{1-y}{1-x}) - 2\,\mathrm{Li}_5(\tfrac{y(1-x)}{x(1-y)}) + \\ & - 2\,\mathrm{Li}_5(x) - \mathrm{Li}_5(1-\tfrac{1}{x}) + S_{3,2}(x) + \\ & - 2\,\mathrm{Li}_5(y) - \mathrm{Li}_5(1-\tfrac{1}{y}) + S_{3,2}(y)\,. \end{aligned}$$

Notice here that the other leading terms arise from symmetrising $-2\,\mathrm{Li}(\frac{x}{y})$ under the 3-fold symmetry $(x,y) \mapsto (1-\frac{1}{x}, 1-\frac{1}{y})$ which manifests on the left hand side. We can make this symmetry fully manifest on the right hand side too, at the expense of using a large number of Nielsen terms.

Identity 4.2.10. *The following, fully symmetric, identity holds modulo products.*

$$\begin{aligned} I_{4,1}(x,y) + I_{4,1}(1-\tfrac{1}{x}, 1-\tfrac{1}{y}) + I_{4,1}(\tfrac{1}{1-x}, \tfrac{1}{1-y}) \overset{⧢}{=} {} & -2\left(\mathrm{Li}_5(\tfrac{x}{y}) + \mathrm{Li}_5(\tfrac{1-y}{1-x}) + \mathrm{Li}_5(\tfrac{y(1-x)}{x(1-y)})\right) + \\ - \mathrm{Li}_5(x) - \mathrm{Li}_5(1-\tfrac{1}{x}) - \mathrm{Li}_5(\tfrac{1}{1-x}) + \frac{1}{3}\bigg(& S_{3,2}(x) + S_{3,2}(1-\tfrac{1}{x}) + S_{3,2}(\tfrac{1}{1-x})\bigg) + \\ - \mathrm{Li}_5(y) - \mathrm{Li}_5(1-\tfrac{1}{y}) - \mathrm{Li}_5(\tfrac{1}{1-y}) + \frac{1}{3}\bigg(& S_{3,2}(y) + S_{3,2}(1-\tfrac{1}{y}) + S_{3,2}(\tfrac{1}{1-y})\bigg) \end{aligned}$$

Or more compactly,

$$\begin{aligned} \mathrm{Cyc}_{\{a,b,c\}} I_{4,1}((abc)de) \overset{⧢}{=} \mathrm{Cyc}_{\{a,b,c\}} \Bigg(& -2\,\mathrm{Li}_5(bade) + \\ & - \mathrm{Li}_5(abcd) + \tfrac{1}{3} S_{3,2}(abcd) - \mathrm{Li}_5(abce) + \tfrac{1}{3} S_{3,2}(abce)\Bigg)\,. \end{aligned}$$

In particular, we have the following identities for Nielsen polylogarithms from which the above symmetrisation can be built.

Identity 4.2.11. *The following identities hold modulo products, expressing combinations of weight 5 Nielsen's in terms of* Li_5*'s.*

$$\begin{aligned} S_{3,2}(x) + S_{3,2}(\tfrac{1}{x}) &\overset{⧢}{=} 3\,\mathrm{Li}_5(x) \\ S_{3,2}(x) + S_{3,2}(1-x) &\overset{⧢}{=} \mathrm{Li}_5(x) + \mathrm{Li}_5(\tfrac{1}{1-x}) + \mathrm{Li}_5(1-\tfrac{1}{x})\,. \end{aligned}$$

4.2.1.4 Rank of relations for $I_{4,1}$ modulo δ

By considering the relations arising under all permutations of the arguments *abcde*, we obtain the following table which counts the number of linearly independent relations arising from each initial relation.

$I_{4,1}$ relation	Number of terms	Rank of relations
Equation 4.2.1a	2	60
Equation 4.2.1b	2	60
Equation 4.2.2	3	40
Overall rank		100

4.2.2 Relations for $I_{3,2}$ modulo δ, and the connection to $I_{4,1}$

4.2.2.1 Symmetries of $I_{3,2}$ modulo δ

As hinted at above, in Equation 4.2.1b and Section 4.2.1.2, we expect a symmetry from inverting the arguments. Indeed we have this.

Identity 4.2.12. *Modulo δ, the following symmetry holds for $I_{3,2}$.*

$$I_{3,2}((ab)cde) \overset{\delta}{=} -I_{3,2}((ba)cde)\,, \tag{4.2.4}$$

or equivalently

$$I_{3,2}(x,y) \overset{\delta}{=} -I_{3,2}(\tfrac{1}{x},\tfrac{1}{y})\,. \tag{4.2.4$'$}$$

As previously, we can find the Li_5 terms which make this identity hold exactly modulo products. We find

Identity 4.2.13. *Modulo $⧢$, the following identity holds for $I_{3,2}$*

$$I_{3,2}(x,y) + I_{3,2}(\tfrac{1}{x},\tfrac{1}{y}) \overset{⧢}{=} \mathrm{Li}_5\left(-[x] + 4[y] + 6\left[\tfrac{x}{y}\right]\right)$$

This is the only simple symmetry of $I_{3,2}$, but other relations do hold modulo δ.

4.2.2.2 Other relations for $I_{3,2}$ modulo δ

A certain 'symmetrisation' of 2-term identities swapping $x \leftrightarrow y$ (equivalently $d \leftrightarrow e$) does hold.

Identity 4.2.14. *Modulo δ, the following 4-term relation holds*

$$I_{3,2}(ab(d)c(e)) - I_{3,2}(ab(e)c(d)) \overset{\delta}{=} -(I_{3,2}(abc(de)) - I_{3,2}(abc(ed)))\,. \tag{4.2.5}$$

So that $I_{3,2}(abc(de)) - I_{3,2}(abc(ed))$ is antisymmetric under swapping $c \leftrightarrow d$.

Or equivalently

$$I_{3,2}(ab(cd)e) + I_{3,2}(ab(dc)e) \overset{\delta}{=} I_{3,2}((ab(ce)d) + I_{3,2}(ab(ec)d)\,,$$

so that $I_{3,2}(ab(cd)e) + I_{3,2}(ab(dc)e)$ *is symmetric under swapping* $d \leftrightarrow e$.

Similarly a 'symmetrisation' of the 3-term 'cyclic' identity for $I_{4,1}$ holds.

Identity 4.2.15. *Modulo* δ*, the following 6-term relation hold*

$$\mathrm{Cyc}_{\{\,a,b,c\,\}}\, I_{3,2}((abc)de) \overset{\delta}{=} -\,\mathrm{Cyc}_{\{\,a,b,c\,\}}\, I_{3,2}((abc)ed)\,, \tag{4.2.6}$$

so that $\mathrm{Cyc}_{\{\,a,b,c\,\}}\, I_{3,2}((abc)de)$ *is anti-symmetric under* $d \leftrightarrow e$.

Knowing some ways to relate $I_{3,2}$, and $I_{4,1}$, these relations are not at all surprising. And moreover, it becomes easy to add the missing Li_5 terms to get identities holding modulo $\sqcup\!\sqcup$.

4.2.2.3 Relating $I_{4,1}$ and $I_{3,2}$, and consequences for $I_{3,2}$ identities

We can express certain combinations of $I_{3,2}$ in terms of $I_{4,1}$, as indicated.

Identity 4.2.16. *Modulo* $\sqcup\!\sqcup$*, we have*

$$\mathrm{Cyc}_{\{\,c,d\,\}}\, I_{3,2}(ab(cd)e) \overset{\sqcup\!\sqcup}{=} -\Big(\mathrm{Cyc}_{\{\,c,d,e\,\}}\, I_{4,1}(ab(cde))\Big) + 2\,\mathrm{Li}_5(bade) - 4\,\mathrm{Li}_5(abcd) + 2\,\mathrm{Li}_5(abce) \tag{4.2.7a}$$

$$\mathrm{Cyc}_{\{\,d,e\,\}}\, I_{3,2}(abc(de)) \overset{\sqcup\!\sqcup}{=} -3 I_{4,1}(abcde)\,. \tag{4.2.7b}$$

Most interesting is the second equation above Equation 4.2.7b, which expressed a single $I_{4,1}$ term in terms of $I_{3,2}$. This gives us a way to eliminate the index 1 from a depth 2 iterated integral; we will make use of this later Section 5.3 to reduce $I_{1,1,1,1,1}$ to $I_{3,2}$ terms. It is worth asking whether a similar conversion expressing one $I_{3,2}$ term as a sum of $I_{4,1}$'s is possible.

$I_{3,2}$ in terms of $I_{4,1}$: Perhaps surprisingly, it is *not* possible to express $I_{3,2}(abcde) = I_{3,2}(x,y)$ using terms of the form $I_{4,1}(abcde)$ with our 'coupled' cross-ratio arguments. However, a much more brute-force route does lead to such an expression. Modulo δ, we compute $I_{4,1}(x,y)$ and $I_{3,2}(x,y)$ to be as follows

$$I_{4,1}(x,y) \overset{\delta}{=} -\{x\}_2 \wedge \{y\}_3 + \{x\}_3 \wedge \{y\}_2 \tag{4.2.8}$$

$$I_{3,2}(x,y) \overset{\delta}{=} \{x\}_2 \wedge \left\{\tfrac{x}{y}\right\}_3 - \{y\}_2 \wedge \left\{\tfrac{x}{y}\right\}_3 + 2\,\{x\}_2 \wedge \{y\}_3 + \{y\}_2 \wedge \{x\}_3 \tag{4.2.9}$$

Since $\mathrm{Li}_3(x) \overset{\sqcup\!\sqcup}{=} \mathrm{Li}_3(\frac{1}{x})$, we have $\{x\}_3 = \left\{\frac{1}{x}\right\}_3$. Therefore, using this we get

$$I_{4,1}(x,y) + I_{4,1}(x,\tfrac{1}{y}) \overset{\delta}{=} 2\,\{x\}_2 \wedge \{y\}_3\,.$$

This combination of integrals will occur again in Chapter 7, when we look at Goncharov's approach to finding highly generic functional equations for Li_5. We can now write every term appearing $I_{3,2}(x,y)$ mod δ directly in terms of $I_{4,1}$ to obtain the following.

Identity 4.2.17. *Modulo δ, we can express the single term $I_{3,2}(x,y)$ using $I_{4,1}$ as follows.*

$$I_{3,2}(x,y) \overset{\delta}{=} -\frac{1}{2}\Big(3I_{4,1}(x,y) + I_{4,1}(x,\tfrac{1}{y}) + I_{4,1}(x,\tfrac{x}{y}) + \\ + I_{4,1}(x,\tfrac{y}{x}) - I_{4,1}(y,\tfrac{x}{y}) - I_{4,1}(y,\tfrac{y}{x})\Big)$$

It would be desirable to find the Li_5 terms which make this identity hold modulo $\sqcup\!\sqcup$. Using Danylo Radchenko's sage package MESA [MESA] to search for 'good' Li_5 arguments, I find that it is possible to do this. However, the resulting terms Li_5 arguments are significantly more complicated than one might initially expect. Moreover, the identity itself is very long. The resulting identity is presented in Section B.1.

Returning to the original conversions between $I_{3,2}$ and $I_{4,1}$ from Identity 4.2.16, it becomes clear that Identity 4.2.14 and Identity 4.2.15 follow from their counterparts for $I_{4,1}$. We have

Explanation of Identity 4.2.14. Consider the left hand side of Equation 4.2.14. We have

$$\begin{aligned} I_{3,2}(ab(cd)e) + I_{3,2}(ab(dc)e) &\overset{\delta}{=} \mathrm{Cyc}_{\{\,c,d\,\}}\, I_{3,2}(ab(cd)e) \\ &\overset{\delta}{=} -\mathrm{Cyc}_{\{\,c,d,e\,\}}\, I_{4,1}(ab(cde))\,. \end{aligned}$$

Using the cyclic invariance now, we can write this as

$$\begin{aligned} &\overset{\delta}{=} -\mathrm{Cyc}_{\{\,e,c,d\,\}}\, I_{4,1}(ab(ecd)) \\ &\overset{\delta}{=} \mathrm{Cyc}_{\{\,e,c\,\}}\, I_{3,2}(ab(ec)d) \\ &\overset{\delta}{=} I_{3,2}(ab(ec)d) + I_{3,2}(ab(ce)d)\,. \end{aligned}$$

But this is just the right hand side of Equation 4.2.14. □

Explanation of Identity 4.2.15. The difference between the left hand side and the right hand side of Equation 4.2.6 can be written as

$$\mathrm{Cyc}_{\{\,a,b,c\,\}}\, \mathrm{Cyc}_{\{\,d,e\,\}}\, I_{3,2}((abc)(de))\,,$$

but using Equation 4.2.7b, this is just

$$\overset{\delta}{=} -3\,\mathrm{Cyc}_{\{\,a,b,c\,\}}\, I_{4,1}((abc)de)\,.$$

And this vanishes modulo δ using Identity 4.2.3. □

Keeping track of the Li_5 terms throughout and using the corresponding $I_{4,1}$ identities from Identity 4.2.10 and Identity 4.2.7 means we can complete Identity 4.2.14 and Identity 4.2.15 to the following identities holding modulo $\sqcup\!\sqcup$.

Identity 4.2.18. *Modulo $\sqcup\!\sqcup$ the following identities hold on $I_{3,2}$.*

$$I_{3,2}(ab(cd)e) + I_{3,2}(ab(dc)e) - I_{3,2}((ab(ce)d) - I_{3,2}(ab(ec)d) \overset{\sqcup\!\sqcup}{=} -6\,\mathrm{Li}_5(abcd) + 6\,\mathrm{Li}_5(abce)$$

$$\begin{aligned}\mathrm{Cyc}_{\{\,a,b,c\,\}}\, I_{3,2}(abc(de)) - I_{3,2}(abc(ed)) &\overset{\sqcup\!\sqcup}{=} 6\,\mathrm{Li}_5(bade) + 6\,\mathrm{Li}_5(cbde) + 6\,\mathrm{Li}_5(acde) + \\ &+ 6\,\mathrm{Li}_5(abcd) + 3\,\mathrm{Li}_5(bcad) - 3S_{3,2}(abcd) + \\ &+ 6\,\mathrm{Li}_5(abce) + 3\,\mathrm{Li}_5(bcae) - 3S_{3,2}(abce)\end{aligned}$$

An amusing way to phrase the two identities in Identity 4.2.16, along with Identity 4.2.13, is the following.

Proposition 4.2.19. *Modulo* δ and $I_{4,1}$ *terms, the iterated integral* $I_{3,2}(abcde)$ *is*

- *antisymmetric in cde, and*
- *symmetric in ab.*

4.2.2.4 An 'exceptional' $I_{3,2}$ identity

The identities from Identity 4.2.13, Equation 4.2.14, and Identity 4.2.15 describe nearly all of the identities that hold between the terms $I_{3,2}(abcde)$. Altogether they describe 90 out of the 91 identities which hold. However one final identity is missing from this list.

To describe this identity it is convenient to briefly introduce some new notation as follows. Let

$$S(abcde) \coloneqq \mathrm{Cyc}_{\{\,a,b,c\,\}}\, I_{3,2}(abcde) = I_{3,2}(abcde) + I_{3,2}(bcade) + I_{3,2}(cabde)\,.$$

Then we have the following identity.

Identity 4.2.20. *Modulo* δ*, we have the following* 3×10*-term identity.*

$$\mathrm{Cyc}_{\{\,a,b,c,d,e\,\}}\, S(abcde) \overset{\delta}{=} \mathrm{Cyc}_{\{\,a,c,e,b,d\,\}}\, S(acebd)\,. \tag{4.2.10}$$

On the right hand side the parameters in the argument step by 2 each time, whereas on the the left hand side the parameters step by 1. So one can view this identity as equating $\mathrm{Cyc}_\bullet\, S((abcde)^p)$ for various choices of p ($p = 1$ and $p = 2$ above) where $(abcde)$ is interpreted as a 5-cycle.

We can lift this to an identity holding modulo ⧢, using Li_5 and Nielsen terms.

Identity 4.2.21. *Modulo* ⧢*, the following 30 term identity on* $I_{3,2}$ *holds*

$$\begin{aligned}&\mathrm{Cyc}_{\{\,a,b,c,d,e\,\}}\, S(abcde) - \mathrm{Cyc}_{\{\,a,c,e,b,d\,\}}\, S(acebd) \overset{\sqcup\!\sqcup}{=} \\ &\quad 3\,\mathrm{Li}_5(-7[abcd] - 3[abce] + 5[abde] + [acbd] + [acbe] + \\ &\quad - 3[acde] - 3[adbc] - 5[adbe] + [adce] + 11[aebc] + \\ &\quad - 9[aebd] + 11[aecd] + 5[bcde] - 5[bdce] - 9[becd]) + \\ &\quad + 18S_{3,2}([abcd] - [aebc] + [aebd] - [aecd] + [becd])\end{aligned}$$

4.2.2.5 Rank of $I_{3,2}$ relations modulo δ

By considering the relations arising under all permutations of the arguments *abcde*, we obtain the following table, which counts the number of linearly independent relations arising from each initial relation.

$I_{3,2}$ relation	Number of terms	Rank of relations
Equation 4.2.4	2	60
Equation 4.2.5	4	40
Equation 4.2.6	6	20
Equation 4.2.10	30	18
Overall rank		91

4.2.3 The remaining depth 2 iterated integrals $I_{2,3}$ and $I_{1,4}$ modulo δ

Having fully analysed the symmetries and relations of $I_{4,1}$ and $I_{3,2}$ modulo δ, including relations between the two different integrals, the remaining cases are not so interesting. Using the stuffle product of multiple polylogarithims, we have the following identities relating $I_{a,b}$ and $I_{b,a}$.

Proposition 4.2.22. *The following identity holds exactly for any depth 2 iterated integral.*

$$I_{a,b}(x,y) + I_{b,a}(x, \tfrac{x}{y}) = I_{a,b}(x) + I_b(y) I_a(\tfrac{x}{y})\,.$$

Proof. This is a direct consequence of the stuffle product $*$ of the corresponding multiple polylogarithms. Converting back via Theorem 3.1.5, we have

$$I_a(x) = -\operatorname{Li}_a(\tfrac{1}{x})\,,$$

so that

$$\begin{aligned} I_b(y) I_a(\tfrac{x}{y}) &= \operatorname{Li}_a(\tfrac{1}{y}) * \operatorname{Li}_b(\tfrac{y}{x}) \\ &= \operatorname{Li}_{b,a}(\tfrac{1}{y}, \tfrac{y}{x}) + \operatorname{Li}_{a,b}(\tfrac{y}{x}, \tfrac{1}{y}) + \operatorname{Li}_{a+b}(\tfrac{1}{y}\tfrac{y}{x}) \\ &= \operatorname{Li}_{b,a}(\tfrac{1}{y}, \tfrac{y}{x}) + \operatorname{Li}_{a,b}(\tfrac{y}{x}, \tfrac{1}{y}) + \operatorname{Li}_{a+b}(\tfrac{1}{x})\,. \end{aligned}$$

Now convert to iterated integrals using Theorem 3.1.5 to say

$$\operatorname{Li}_{a,b}(x,y) = I_{a,b}(\tfrac{1}{xy}, \tfrac{1}{y})\,.$$

So we obtain

$$= I_{b,a}(x, \tfrac{x}{y}) + I_{a,b}(x,y) - I_{a+b}(x)\,.$$

Rearranging this gives the desired equality. □

In terms of the cross-ratio arguments, this means we have

$$I_{n,m}(abcde) \overset{ш}{=} -I_{m,n}(badce) - \operatorname{Li}_{n+m}(bacd)\,,$$

so that identities for $I_{3,2}$ modulo δ can be translated to directly to identities for $I_{2,3}$, and vice-versa. Similarly for $I_{4,1}$ identities and $I_{1,4}$ identities. So there is no need to analyse the cases $I_{2,3}$ and $I_{1,4}$ in detail.

4.3 Depth 3 iterated integrals

At depth 3, there are many more integrals to consider: $I_{3,1,1}$, $I_{1,3,1}$, $I_{1,1,3}$, $I_{2,2,1}$, $I_{2,1,2}$ and $I_{1,2,2}$. Therefore, there are many more potential relations between different integrals to be investigated. The simplest integral here appears to be $I_{3,1,1}$, so this is a good place to start.

4.3.1 Relations for $I_{3,1,1}$ modulo δ

The integral $I_{3,1,1}(abcdef)$ has no straight-forward symmetries, but perhaps the simplest relation for $I_{3,1,1}$ is the following, which has the form not dissimilar to the 2-term inversion relations that hold for $I_{a,b}(\frac{1}{x}, \frac{1}{y})$. Specifically we have

Identity 4.3.1. *Modulo δ the following 4-term relation holds*

$$\mathrm{Cyc}_{\{\,a,b\,\}}\, I_{3,1,1}((ab)(cdef)) \overset{\delta}{=} \mathrm{Cyc}_{\{\,a,b\,\}}\, I_{3,1,1}((ab)(fedc))\,.$$

From the left hand side to the right hand side there is a reversal of $cdef$.

Of course, we can find the Li_5 terms, to obtain a more precise identity.

Identity 4.3.2. *Modulo $⧢$, the following relation holds*

$$\mathrm{Cyc}_{\{\,a,b\,\}}\left(I_{3,1,1}((ab)(cdef)) - I_{3,1,1}((ab)(fedc))\right) \overset{⧢}{=} \mathrm{Li}_5\left(-4[badf] + [baef] + 4[abce] - [abcd]\right)\,.$$

The next simplest identity, linearly independent from the previous, appears to be an 8-term relation of the following form, which already holds modulo products.

Identity 4.3.3. *Modulo δ, and in fact already modulo $⧢$, the following 8-term relation holds.*

$$\mathrm{Alt}_{\{\,c,e\,\}}\,\mathrm{Alt}_{\{\,d,f\,\}}\left(I_{3,1,1}((ab)(cdef)) - I_{3,1,1}((ba)(fedc)\right) \overset{⧢}{=} 0\,.$$

By successively taking new identities, linearly independent from any of the previous, we obtain a sequence of increasingly complicated identities, with an increasing number of terms.

For example, we find a 16 term identity.

Identity 4.3.4. *Modulo δ the following 16-term relation holds.*

$$\begin{aligned}&\mathrm{Alt}_{\{\,c,d\,\}}\, I_{3,1,1}(-[abdefc] - [abdfce] - [abdfec] + [abedfc] + \\ &+ [abfdec] + [badecf] + [badfce] - [baedfc]) \overset{\delta}{=} 0\end{aligned}$$

Then we find a 24 term, a 36 term, a 48 term identity, and so on. It turns out that each of these has a non-trivial Li_5 component.

The most generic (and most complicated) of all identities for $I_{3,1,1}$ modulo δ appears to be a 152-term identity, which involves only coefficients ± 1, ± 2. This 152-term identity generates a 522 dimensional space, but already this exhausts all relations on $I_{3,1,1}$ modulo δ. Necessarily, since Identity 4.3.2 has a non-trivial Li_5 component and this 152-term identity implies it, the 152-term identity has a non-trivial Li_5 component.

The description of the $I_{3,1,1}$ relations modulo δ is rather more complicated than the corresponding description for the depth 2 integrals. This suggests that maybe we have been *too* restrictive in the choice of arguments, or the depth we work modulo.

4.3.2 Relations for $I_{3,1,1}$ modulo $I_{3,2}$

Allowing only identities which hold between $I_{3,1,1}$ terms with cross-ratio arguments, modulo δ is perhaps *too* restrictive. We should consider identities which involve lower depth terms beyond Li_5.

However, it does not make sense to ask for identities holding modulo depth 2, since every iterated integral of weight 5 is expected to be expressible in terms of depth ≤ 2 iterated integrals. But perhaps we can still find some interesting results by asking for combinations of $I_{3,1,1}$ which can be expressed in terms of depth 2 integrals with the 'simple' cross-ratio arguments. From Identity 4.2.16 and Section 4.2.3 we know how to express every depth 2 iterated integral in terms of $I_{3,2}$, so it suffices to consider only $I_{3,2}$.

Henceforth, we introduce the following notation.

Notation 4.3.5. We will write $\overset{I_{3,2}}{=}$ to indicate results which hold modulo δ and *explicit* $I_{3,2}(abcde)$ terms, with these simple cross-ratio arguments.

Modulo $I_{3,2}$, the integral $I_{3,1,1}$ satisfies a number of genuine symmetries, namely we have the following.

Identity 4.3.6. *The following symmetries hold modulo $I_{3,2}$.*

$$I_{3,1,1}((ab)cdef) \overset{I_{3,2}}{=} I_{3,1,1}((ba)cdef) \tag{4.3.1}$$

$$I_{3,1,1}(ab(cdef)) \overset{I_{3,2}}{=} I_{3,1,1}(ab(fedc)) \tag{4.3.2}$$

Indeed, these are the only symmetries of $I_{3,1,1}$ modulo $I_{3,2}$.

The next simplest identities which appear are 4-term identities.

Identity 4.3.7. *The following 4-term identities for $I_{3,1,1}$ hold modulo $I_{3,2}$.*

$$\mathrm{Cyc}_{(bc)(ef)}\, I_{3,1,1}(a(bc)d(ef)) \overset{I_{3,2}}{=} \mathrm{Cyc}_{(bc)(ef)}\, I_{3,1,1}(d(ef)a(bc)) \tag{4.3.3}$$

$$\mathrm{Cyc}_{\{\,d,e\,\}}\, I_{3,1,1}(abc(de)f \overset{I_{3,2}}{=} \mathrm{Cyc}_{\{\,d,e\,\}}\, I_{3,1,1}(fcb(de)a) \tag{4.3.4}$$

Moreover, we now obtain two different types of 5-term identities for $I_{3,1,1}$ modulo $I_{3,2}$. Unfortunately the identities appear to lack a nice structure, nevertheless we have the following.

Identity 4.3.8. *Modulo $I_{3,2}$, the following identities hold.*

$$I_{3,1,1}([abcdef] + [acefdb] + [adfcbe] + [aecfbd] + [afdceb]) \overset{I_{3,2}}{=} 0 \tag{4.3.5}$$

$$I_{3,1,1}([abcdef] + [aecfbd] + [caefdb] + [cbeadf] + [cebafd]) \overset{I_{3,2}}{=} 0 \tag{4.3.6}$$

Maybe one would prefer a longer relation that is more structured. In which case, we have also an 8-term relation for $I_{3,1,1}$ modulo $I_{3,2}$.

Identity 4.3.9. *Modulo $I_{3,2}$, the following 8-term relation holds for $I_{3,1,1}$.*

$$\mathrm{Alt}_{\{\, c,d \,\}} \mathrm{Cyc}_{(ae)(bf)} \mathrm{Cyc}_{(bc)(ef)} I_{3,1,1}(abcdef) \overset{I_{3,2}}{=} 0 \tag{4.3.7}$$

It turns out that these identities, Equations 4.3.1 to 4.3.7, are already more than enough to generate *all* 687 relations on $I_{3,1,1}$ modulo $I_{3,2}$. The description of all $I_{3,1,1}$ relations modulo $I_{3,2}$ is much simpler than the corresponding description modulo δ, but not trivially so. This confirms that looking modulo $I_{3,2}$ is a good idea.

4.3.2.1 Rank and bases of $I_{3,1,1}$ relations modulo $I_{3,2}$

By considering the relations arising under all permutations of the arguments $abcdef$, we obtain the following table which counts the number of linearly independent relations arising from each initial relation.

$I_{3,1,1}$ relation	Number of terms	Rank of relations
Equation 4.3.1	2	360
Equation 4.3.2	2	360
Equation 4.3.3	4	180
Equation 4.3.4	4	180
Equation 4.3.5	5	432
Equation 4.3.6	5	672
Equation 4.3.7	8	180
Overall rank		687

We can take any of the following choices to obtain a 'minimal' basis for the $I_{3,1,1}$ relations, modulo $I_{3,2}$

$I_{3,1,1}$ relation	Number of terms	Bases						
Equation 4.3.1	2							
Equation 4.3.2	2	✓				✓		
Equation 4.3.3	4		✓			✓	✓	
Equation 4.3.4	4			✓				✓
Equation 4.3.5	5					✓	✓	✓
Equation 4.3.6	5	✓	✓	✓	✓			
Equation 4.3.7	8				✓		✓	✓

4.3.2.2 $I_{3,2}$, Li_5 and Nielsen terms for $I_{3,1,1}$ relations holding modulo $I_{3,2}$

We can lift the identities in Equations 4.3.1 to 4.3.6, to identities holding modulo δ (and potentially even modulo $\shuffle$), by finding explicit $I_{3,2}$ and Li_5 terms.

Identity 4.3.10. *We can find $I_{3,2}$ and Li_5 terms for Equation 4.3.2 and Equation 4.3.1 to give the following identities which holds modulo $\shuffle$.*

$$I_{3,1,1}(ab(cdef)) - I_{3,1,1}(ab(cdef)) \overset{\shuffle}{=} I_{3,2}(abcde) - I_{3,2}(abfed)$$

$$\begin{aligned} I_{3,1,1}((ab)cdef) - I_{3,1,1}((ba)cdef]) \overset{\shuffle}{=} & \frac{1}{3} I_{3,2}(3[abcde] - [abcdf] - 2[abcef] - [abcfd] + \\ & + [abcfe] - 2[abecf] + [abefc] - 3[abfed]) + \\ & + \mathrm{Li}_5([abcd] - 4[abce] + 3[abcf] + 4[badf] + 2[baef]) \,. \end{aligned}$$

The first 5-term identity, Equation 4.3.5 is very easy to lift to an identity modulo products, for we have the following.

Identity 4.3.11. *We can find $I_{3,2}$ and Li_5 terms for Equation 4.3.5 to give the following identity which holds modulo $\shuffle$.*

$$\begin{aligned} & I_{3,1,1}([abcdef] + [acefdb] + [adfcbe] + [aecfbd] + [afdceb]) \overset{\shuffle}{=} \\ & \quad - I_{3,2}([facbd] + [fbdac] + [fcabe] + [fdbae] + [feadc]) + \\ & \quad + 6\,\mathrm{Li}_5([acbf] + [aedf] + [afbd] + [becf] + [cdef]) \end{aligned}$$

However, lifting the 4-term identities is already more difficult. They require a large number of $I_{3,2}$ terms. Moreover, $\mathrm{Li}_5(abcd)$ terms are not sufficient; we need to invoke weight 5 Nielsen polygarithms. We have

Identity 4.3.12. *We can find $I_{3,2}$ and Li_5 and Nielsen terms for Equation 4.3.3 to give the following identities which hold modulo $\shuffle$.*

$$\begin{aligned} & I_{3,1,1}([abcdef] + [acbdfe] - [defabc] - [dfeacb]) \overset{\shuffle}{=} \\ & \frac{1}{3} I_{3,2}(-[abdfe] + [abefd] - [acdef] - [acefd] + [acfed] - [aecbf] - [aecfb] + \end{aligned}$$

$$
\begin{aligned}
&- [afbce] - [afbec] + [bafed] - [bdfce] - [bdfec] + [bface] - [bfcae] + \\
&+ [bfcde] + [bfdec] + [bfeac] - [bfedc] - [cdebf] - [cdefb] + [ceabf] + \\
&- [cebaf] + [cebdf] + [cedfb] + [cefab] - [cefdb] + [deacb] - [debca] + \\
&+ [dfabc] + [dfbca] - [dfcba] - [edcba]) + \\
+ \mathrm{Li}_5(&4[abef] - 4[acbe] - 4[acef] + 8[aecf] - 4[afbc] + 4[afbe] + 4[afce] + \\
&- 4[bcde] + 4[bcef] + 4[bdce] - 4[bdcf] + 4[bdef] + 4[bfcd] - 4[bfce] + \\
&- 4[cfde] + [abcf] - \tfrac{4}{3}[abdf] - \tfrac{5}{3}[abef] + 3[acbe] - [acbf] + \tfrac{4}{3}[acde] + \\
&+ 2[acef] + [adbc] - [adef] - [aebc] + 3[aebf] - 3[aecf] + 2[afbc] + \\
&- [afbe] + [afce] + \tfrac{2}{3}[bcde] - [bcdf] - 2[bcef] + 3[bdcf] - [bdef] + \\
&- [becf] - [bedf] - [bfcd] - [bfce] - [bfde] + 2[cdef] - 2[cedf] + 2[cfde]) + \\
+ S_{3,2}(&-[abef] + [acbe] + [acef] - 2[aecf] + [afbc] - [afbe] - [afce] + [bcde] + \\
&- [bcef] - [bdce] + [bdcf] - [bdef] - [bfcd] + [bfce] + [cfde])
\end{aligned}
$$

Identity 4.3.13. *We can find $I_{3,2}$ and Li_5 and Nielsen terms for Equation 4.3.4 to give the following identities which hold modulo ш.*

$$
\begin{aligned}
&I_{3,1,1}([abcdef] + [abcedf] - [fcbdea] - [fcbeda]) \overset{ш}{=} \\
&\frac{1}{3} I_{3,2}([abcde] + [abced] - [abfde] - [abfed] + [acbde] - [acbdf] + [acbed] + \\
&\quad - [acbef] - [acbfd] - [acbfe] + [acfed] - [afbcd] - [afbce] - [afbdc] + \\
&\quad - [afbec] - [afcbd] - [afcbe] - [afcdb] - [afceb] + [bfade] + [bfaed] + \\
&\quad - [bfcad] - [bfcae] - [bfcda] + [bfcde] - [bfcea] + [bfced] - [cafde] + \\
&\quad - [cfade] - [cfaed] + [cfbde] + [cfbed]) + \\
&+ \mathrm{Li}_5([abcf] - 5[abde] + [abdf] + [abef] - 4[acbf] + 2[acde] - \tfrac{2}{3}[acdf] + \\
&\quad - \tfrac{10}{3}[acef] - [adbe] - 2[adbf] - 2[adcf] - [aebd] - 2[aebf] - 3[aecf] + \\
&\quad - 4[afbc] - 4[afbd] - 4[afbe] - 4[afcd] - 5[afce] + [bdcf] - 2[bdef] + \\
&\quad + [becf] + [bedf] + 5[bfde] - 2[cdef] + [cedf] + 5[cfde]) + \\
&+ S_{3,2}(-[abde] - [acbf] - [acef] - [adbe] - [aecf] - [afbc] - [afbd] + \\
&\quad - [afbe] - [afcd] - [afce] - [bdef] + [bfde] - [cdef] + [cfde])
\end{aligned}
$$

Similarly, lifting the second 5-term identity, Equation 4.3.6, to an identity modulo δ is difficult. The shortest expression I find for it, modulo δ, already involves a sum of 41 $I_{3,2}$ terms.

Identity 4.3.14. *We can find $I_{3,2}$, Li_5 and Nielsen terms for Equation 4.3.6, to give the following identity which holds modulo ш.*

$$
I_{3,1,1}([abcdef] + [aecfbd] + [caefdb] + [cbeadf] + [cebafd]) \overset{ш}{=}
$$

$$\frac{1}{3} I_{3,2}([acbde] + [acbed] - [acdef] + [acebf] + [acefb] - [acefd] + [acfed] +$$
$$- [aecfd] + [badfe] - [baefd] + [bafed] + [bcafd] - [bcdfa] + [bcfda] +$$
$$+ [bfced] + [daebc] + [daecb] + [dcebf] + [dcefb] - [deafb] - [debaf] +$$
$$+ [debcf] + [defab] - [defcb] - [eabdf] + [eacdf] + [eadbf] + [eafdb] +$$
$$- [ecafd] + [ecdfa] - [ecfda] + [edcbf] + [fabce] + [fabec] - [fbade] +$$
$$+ [fbdae] - [fbdce] - [fbead] + [fbecd] + [fcbde] + [fcbed])+$$
$$+ \mathrm{Li}_5(3[daec] - [dbea] + [dcbe] - \frac{1}{3}[dcea] + 2[deac] + [deba] - \frac{10}{3}[debc]] +$$
$$+ 3[fabc] + 2[fadb] + 5[fbac] + \frac{19}{3}[fbdc] + [fbea] - \frac{10}{3}[fbec] + [fcba]] +$$
$$+ [fcbe] + [fcdb] + \frac{19}{3}[fcde] + \frac{1}{3}[fcea] - 3[fdac] - 2[fdec] - 2[feac]] +$$
$$- [feba] + 2[feda] + [fedc]) +$$
$$+ S_{3,2}([daec] - [dbea] + [deba] - [debc] + [fabc] + [fadb] + [fbac] +$$
$$+ 2[fbdc] + [fbea] - [fbec] + 2[fcde] - [feac] - [feba] + [feda]) \, .$$

4.3.3 A simple way to relate depth 3 integrals, modulo ⧢

We observed in the case $I_{2,3}$ that some of the depth 2 integrals can be directly related. A similar phenomenon happens for depth 3 iterated integral. Namely we have the following proposition, which is a variant of Proposition 4.2.5, in depth 3.

Proposition 4.3.15. *The following identity on iterated integrals holds exactly.*

$$I_{a,b,1}(x,y,z) - (-1)^{a+b} I_{b,a,1}(z,y,x) =$$
$$- \sum_{i=1}^{b} (-1)^i I_i(z) I_{a,b+1-i}(x,y) - (-1)^{a+b} \sum_{i=1}^{a} (-1)^i I_i(x) I_{b,a+1-i}(z,y)$$

Proof. As in Proposition 4.2.5, we translate the identity to an identity on words describing differential forms. I claim the following sum of words evaluates as indicated

$$\sum_{i=1}^{b} (-1)^i (x0^{i-1}) ⧢ (z0^{a-1}y0^{b-i}) = -(x0^{b-1} ⧢ z0^{a-1})y + (-1)^b (z0^{a-1}y0^{b-1}x)$$

The cases $b = 1$, and $b = 2$ are just an easy check by expanding out all the shuffle products. So take $b > 2$. Then

$$\sum_{i=1}^{b} (-1)^i (x0^{i-1}) ⧢ (z0^{a-1}y0^{b-i})$$
$$= \sum_{i=2}^{b-1} (-1)^i (x0^{i-1}) ⧢ (z0^{a-1}y0^{b-i}) - x ⧢ (z0^{a-1}y0^{b-1}) + (-1)^b x0^{b-1} ⧢ (z0^{a-1}y)$$
$$= \sum_{i=2}^{b-1} (-1)^i ((x0^{i-2}) ⧢ (z0^{a-1}y0^{b-i}))0 + (-1)^i ((x0^{i-1}) ⧢ (z0^{a-1}y0^{b-(i+1)}))0 +$$

$$- x \sqcup\!\sqcup (z0^{a-1}y0^{b-1}) + (-1)^b(x0^{b-1}) \sqcup\!\sqcup (z0^{a-1}y)\,,$$

by expanding out the shuffle product using the iterative definition which removes the last letters.

Now this is

$$\begin{aligned}
&= \sum_{i=2}^{b-1}(-1)^i((x0^{i-2}) \sqcup\!\sqcup (z0^{a-1}y0^{b-i}))0 - \sum_{i=2}^{b-1}(-1)^{i+1}((x0^{(i+1)-2}) \sqcup\!\sqcup (z0^{a-1}y0^{b-(i+1)}))0 \\
&\quad - x \sqcup\!\sqcup (z0^{a-1}y0^{b-1}) + (-1)^b(x0^{b-1}) \sqcup\!\sqcup (z0^{a-1}y)\,.
\end{aligned}$$

But only the $i = 2$ term of the first sum, and the $i = b - 1$ term of the second sum survive, giving

$$\begin{aligned}
&= (x \sqcup\!\sqcup (z0^{a-1}y0^{b-2}))0 - (-1)^b((x0^{b-2}) \sqcup\!\sqcup (z0^{a-1}y))0 \\
&\quad - x \sqcup\!\sqcup (z0^{a-1}y0^{b-1}) + (-1)^b(x0^{b-1}) \sqcup\!\sqcup (z0^{a-1}y)\,.
\end{aligned}$$

Using the definition of the shuffle product the vertical pairs can be combined to give

$$\begin{aligned}
&= -(\emptyset \sqcup\!\sqcup (z0^{a-1}y0^{b-1})))x + (-1)^b((x0^{b-1}) \sqcup\!\sqcup (z0^{a-1}))y \\
&= -(z0^{a-1}y0^{b-1}x) + (-1)^b((x0^{b-1}) \sqcup\!\sqcup (z0^{a-1}))y\,.
\end{aligned}$$

So finally, if we consider the following sum of two versions of the previous result, we get

$$\begin{aligned}
&- \sum_{i=1}^{b}(-1)^i(z0^{i-1}) \sqcup\!\sqcup (x0^{a-1}y0^{b-i}) + (-1)^{a+b}\sum_{i=1}^{a}(-1)^i(x0^{i-1}) \sqcup\!\sqcup (z0^{b-1}y0^{a-i}) \\
&= -(-(x0^{a-1}y0^{b-1}z) + (-1)^b((z0^{b-1}) \sqcup\!\sqcup (x0^{a-1}))y) + \\
&\quad + (-1)^{a+b}(-(z0^{b-1}y0^{a-1}x) + (-1)^a((x0^{a-1}) \sqcup\!\sqcup (z0^{b-1}))y) \\
&= (x0^{a-1}y0^{b-1}z) + (-1)^{a+b}(z0^{b-1}y0^{a-1}x)\,.
\end{aligned}$$

So taking integrals of this equality, we obtain the identity we want

$$\begin{aligned}
&I_{a,b,1}(x, y, z) + (-1)^{a+b}I_{b,a,1}(z, y, x) = \\
&- \sum_{i=1}^{b}(-1)^iI_i(z)I_{a,b+1-i}(x, y) - (-1)^{a+b}\sum_{i=1}^{a}(-1)^iI_i(x)I_{b,a+1-i}(z, y)\,.
\end{aligned}$$

This proves the proposition. □

In particular, this proposition allows us to claim the following identities, modulo $\sqcup\!\sqcup$.

Identity 4.3.16. *Taking $a = 1$, and $b = 3$ in Proposition 4.3.15 gives*

$$I_{1,3,1}(x, y, z) \overset{\sqcup\!\sqcup}{=} I_{3,1,1}(z, y, x)\,.$$

Or equivalently, in terms of cross-ratios

$$I_{1,3,1}(abcdef) \overset{\sqcup\!\sqcup}{=} I_{3,1,1}(abcfed)\,.$$

The upshot of this identity is that we can convert directly any identity for $I_{3,1,1}$ modulo $⧢$, δ, or $I_{3,2}$, into a corresponding identity for $I_{1,3,1}$. Therefore, we do not need to analyse this case separately.

Identity 4.3.17. *Taking $a = b = 2$ in Proposition 4.3.15 gives*

$$I_{2,2,1}(x, y, z) \overset{⧢}{=} I_{2,2,1}(z, y, x)\,.$$

Or equivalently, in terms of cross-ratios

$$I_{2,2,1}(abc(d)e(f)) \overset{⧢}{=} I_{2,2,1}(abc(f)e(d))\,. \tag{4.3.8}$$

So we already know that $I_{2,2,1}$ satisfies a *genuine* symmetry modulo $⧢$.

4.3.4 More complicated ways to relate depth 3 integrals, modulo $I_{3,2}$

We know how to directly relate the integrals $I_{1,3,1}$ and $I_{3,1,1}$, using Identity 4.3.16. We can therefore immediately skip the analysis of $I_{3,1,1}$. But after analysing the relations between $I_{1,1,3}$ modulo $I_{3,2}$, *et cetera*, one finds that these integrals all have exactly the same number of relations. This is perhaps unexpected. Moreover, many of the relations have a very similar structure. This very much suggests that all the depth 3 integrals are somehow 'equivalent' modulo $I_{3,2}$.

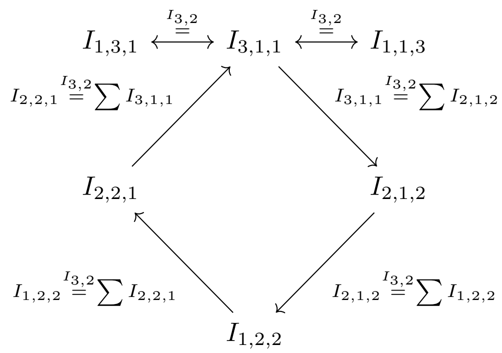
Indeed, this is the case.

Theorem 4.3.18. *Modulo $I_{3,2}$, all of the weight 5, depth 3 iterated integrals span the same space. More precisely, if*

$$\mathcal{B}_f := \left\{ f(\sigma \cdot abcdef) \mid \sigma \in S_{\{\, a,b,c,d,e,f \,\}} \right\}\,,$$

then $\operatorname{span} \mathcal{B}_f$*, modulo $I_{3,2}$, is invariant for $f \in \{ I_{3,1,1}, I_{1,3,1}, I_{1,1,3}, I_{2,2,1}, I_{2,1,2}, I_{1,2,2} \}$.*

Proof. We shall prove this by showing that each $\operatorname{span} \mathcal{B}_f$ equals (for example) $\operatorname{span} \mathcal{B}_{I_{3,1,1}}$, regardless of which integral f is. We shall relate the integral to each other in the following way.



The arrows here express the source integral as a sum of the target integrals, modulo $I_{3,2}$. By following the arrows around, one sees that any integral can be expressed as a sum of any of the other integrals, modulo $I_{3,2}$. Therefore $\operatorname{span} \mathcal{B}_f$ equals $\operatorname{span} \mathcal{B}_{I_{3,1,1}}$, regardless of whcih integral f is.

The proof is nothing more than giving the relevant expressions for $I_{2,2,1}$ as sum of $I_{3,1,1}$'s and $I_{3,2}$'s, and likewise for the remaining cases.

From Identity 4.3.16, we already have

Identity 4.3.16. *Taking $a = 1$, and $b = 3$ in Proposition 4.3.15 gives*

$$I_{1,3,1}(x, y, z) \overset{\sqcup\!\sqcup}{=} I_{3,1,1}(z, y, x)\,.$$

Or equivalently, in terms of cross-ratios

$$I_{1,3,1}(abcdef) \overset{\sqcup\!\sqcup}{=} I_{3,1,1}(abcfed)\,.$$

This deals with expressing $I_{1,3,1}$ in terms of $I_{3,1,1}$, and vice-versa..

For $I_{1,1,3}$ in terms of $I_{3,1,1}$, and vice-versa, we have

Identity 4.3.19.

$$\begin{aligned} I_{3,1,1}(abcdef) - I_{1,1,3}(abdcfe) \overset{\delta}{=} \frac{1}{3} I_{3,2}(&-[abdfe] - [abfce] - [abfde] - [abfed] + \\ &- [baefd] + [bafec] + [bafed])\,. \end{aligned}$$

The expressions relating $I_{3,1,1}$, $I_{2,2,1}$, $I_{2,1,2}$ and $I_{1,2,2}$ are more complicated; with the simple cross-ratio arguments one must relate $I_{3,1,1}$ to a sum of $I_{2,2,1}$'s and vice-versa.

For $I_{2,2,1}$ in terms of $I_{3,1,1}$, we have

Identity 4.3.20.

$$I_{2,2,1}(abcdef) \overset{\sqcup\!\sqcup}{=} -I_{3,1,1}([abcdef] + [abcdfe] + [abcfde] + [abcfed])$$

The remaining identities, expressing $I_{3,1,1}(abcdef)$ as a sum of $I_{2,1,2}$'s, expressing $I_{2,1,2}(abcdef)$ as a sum of $I_{1,2,2}$'s, and expressing $I_{1,2,2}(abcdef)$ as a sum of $I_{2,2,1}$'s are significantly longer. They are presented in Section B.2. □

Remark 4.3.21. This theorem shows immediately that the *number* of identities that each of these depth 3 integrals satisfies is the same, explaining the unexpected observation above. Specifically, the number of relations must equal $\#S_{\{\,a,b,c,d,e,f\,\}} - \dim \operatorname{span} \mathcal{B}_{I_{3,1,1}} = 687$ in each case, since $\operatorname{span} \mathcal{B}_f$ is independent of f.

Moreover, we see that $I_{3,1,1}$, $I_{1,3,1}$ and $I_{1,1,3}$ must satisfy exactly the same identities structurally, since we can exchange these term-for-term modulo $I_{3,2}$. However this is not the case for the remaining integrals because we need to replace each $I_{3,1,1}$ term with a sum of $I_{2,2,1}$'s, for example. And in fact, the structural differences between the $I_{2,2,1}$, $I_{2,1,2}$, $I_{1,2,2}$ and the $I_{3,1,1}$ identities will prove that single terms of these cannot be related, modulo $I_{3,2}$, with coupled cross-ratio arguments.

4.3.5 Identities for $I_{2,2,1}$ modulo $I_{3,2}$

Since we do not have a way to express $I_{2,2,1}(abcdef)$ as a single $I_{3,1,1}$ term, modulo $I_{3,2}$, this integral may satisfy different identities. We should therefore analyse them. It turns out that $I_{2,2,1}$ satisfies a number of relatively short identities, but in order to describe the relations completely it appears that one must invoke longer and longer identities, when compared to the $I_{3,1,1}$ cases. Of the depth 3 integrals, $I_{2,2,1}$ appears to be the most 'complicated' in terms of relations.

$I_{2,2,1}$ satisfies two symmetries modulo $I_{3,2}$. One of them we already know from Identity 4.3.17.

Identity 4.3.17. *Taking $a = b = 2$ in Proposition 4.3.15 gives*

$$I_{2,2,1}(x, y, z) \overset{\sqcup\!\sqcup}{=} I_{2,2,1}(z, y, x)\,.$$

Or equivalently, in terms of cross-ratios

$$I_{2,2,1}(abc(d)e(f)) \overset{\sqcup\!\sqcup}{=} I_{2,2,1}(abc(f)e(d))\,. \tag{4.3.8}$$

The second symmetry is another example of the inverting arguments identity, which can be expressed as a sum of 34 $I_{3,2}$ terms.

Identity 4.3.22. *Modulo $I_{3,2}$, $I_{2,2,1}$ satisfies the following symmetry.*

$$I_{2,2,1}((ab)cdef) \overset{I_{3,2}}{=} I_{2,2,1}((ba)cdef)\,. \tag{4.3.9}$$

Remark 4.3.23. Notice that the first symmetry, Identity 4.3.17, permutes arguments 4 and 6, in the form $I_{2,2,1}(abc(d)e(f))$. This is different from the symmetry $I_{3,1,1}(ab(cdef)) \overset{I_{3,2}}{=} I_{3,1,1}(ab(fedc))$, which permutes arguments $3 \leftrightarrow 6$ and $4 \leftrightarrow 5$. If $I_{2,2,1}(abcdef)$ could be expressed as a single $I_{3,1,1}$ term, modulo $I_{3,2}$, then any symmetry of one integral would translate directly to exactly the same symmetry of the other integral. However, this since the integrals have *different* symmetries, this is not the case. Therefore we cannot express $I_{2,2,1}(abcdef)$ as a single $I_{3,1,1}$ term, modulo $I_{3,2}$.

The next simplest type of identity that $I_{2,2,1}$ satisfies appears to be a 4-term relation.

Identity 4.3.24. *The following 4-term relation holds for $I_{2,2,1}$ modulo $I_{3,2}$.*

$$\mathrm{Cyc}_{(af)(bd)}\,\mathrm{Alt}_{\{\,c,e\,\}}\,I_{2,2,1}(ab(c)d(e)f) \overset{I_{3,2}}{=} 0 \tag{4.3.10}$$

Then $I_{2,2,1}$ satisfies two different 6-term identities, one of which shows a good amount of structure.

Identity 4.3.25. *$I_{2,2,1}$ satisfies the following 6-term relation, modulo $I_{3,2}$.*

$$\mathrm{Alt}_{\{\,c,e\,\}}\,\mathrm{Cyc}_{\{\,c,d,f\,\}}\,I_{2,2,1}(ab(cd)e(f)) \overset{I_{3,2}}{=} 0 \tag{4.3.11}$$

The second 6-term identity does not show much structure, but in place of this it generates a larger number of linearly independent relations.

Identity 4.3.26. *The following 6-term relation for $I_{2,2,1}$ holds modulo $I_{3,2}$*

$$I_{2,2,1}([abcdef] + [aebdfc] - [cdfeba] + [ebafdc] - [fcdeab] - [fdebca]) \overset{I_{3,2}}{=} 0 \tag{4.3.12}$$

Then we have two highly structured 8-term identities.

Identity 4.3.27. *$I_{2,2,1}$ satisfies the following 8-term identities, modulo $I_{3,2}$.*

$$\mathrm{Alt}_{\{\, b,c \,\}}\, \mathrm{Alt}_{\{\, d,e \,\}}\, I_{2,2,1}(a(bc)(de)f) - I_{2,2,1}(f(de)(cb)a) \overset{I_{3,2}}{=} 0 \tag{4.3.13}$$

$$\mathrm{Cyc}_{(ae)(bf)}\, \mathrm{Alt}_{\{\, c,d \,\}}\, \mathrm{Cyc}_{\{\, e,f \,\}}\, I_{2,2,1}(ab(cd)(ef)) \overset{I_{3,2}}{=} 0 \tag{4.3.14}$$

A rather unstructured 10-term identity holds. Unfortunately, it appears that we do need to use it when describing the $I_{2,2,1}$ relations modulo $I_{3,2}$.

Identity 4.3.28. *$I_{2,2,1}$ satisfies the following 10-term identity, modulo $I_{3,2}$.*

$$\begin{aligned} &I_{2,2,1}(+[abcdef] - [abecfd] + [abedcf] - [aebcdf] + [aebdcf]+ \\ &-[fcdbea] + [fcdeba] - [fdcbea] + [fdceab] - [fdebca]) \overset{I_{3,2}}{=} 0 \end{aligned} \tag{4.3.15}$$

The last identity we need to completely describe the null-space is a 15-term identity, which symmetrises the building block of the 6-term relation Identity 4.3.25 in a different way. On top of all of the previous relations, only one instance of the 15-term relation is required.

Identity 4.3.29. *The following 15 term relation holds on $I_{2,2,1}$, modulo $I_{3,2}$*

$$\mathrm{Cyc}_{\{\, b,c,d,e,f \,\}}\, \mathrm{Cyc}_{\{\, c,d,f \,\}}\, I_{2,2,1}(ab(cd)e(f)) \overset{I_{3,2}}{=} 0 \tag{4.3.16}$$

4.3.5.1 Rank and bases of relations for $I_{2,2,1}$ modulo $I_{3,2}$

By considering the relations arising under all permutations of the arguments $abcdef$, we obtain the following table, which counts the number of linearly independent relations arising from each initial relation.

$I_{2,2,1}$ relation	Number of terms	Rank of relations
Equation 4.3.8	2	360
Equation 4.3.9	2	360
Equation 4.3.10	4	180
Equation 4.3.11	6	210
Equation 4.3.12	6	426
Equation 4.3.13	8	90
Equation 4.3.14	8	135
Equation 4.3.15	10	360
Equation 4.3.16	15	144
Overall rank		687

We can take any of the following choices to obtain a 'minimal' basis for the $I_{2,2,1}$ relations modulo $I_{3,2}$.

$I_{2,2,1}$ relation	Number of terms	Bases			
Equation 4.3.8	2	✓			
Equation 4.3.9	2		✓		
Equation 4.3.10	4			✓	
Equation 4.3.11	6				
Equation 4.3.12	6			✓	✓
Equation 4.3.13	8				
Equation 4.3.14	8				✓
Equation 4.3.15	10	✓	✓	✓	✓
Equation 4.3.16	15	✓	✓	✓	✓

4.3.6 Identities for $I_{2,1,2}$ modulo $I_{3,2}$

Next we focus on the integral $I_{2,1,2}$. The relations for $I_{2,1,2}$ seem to be slightly simpler than for $I_{2,2,1}$, intermediate in complexity between $I_{2,2,1}$ and $I_{3,1,1}$.

Differing from any of the previous integrals, the integral $I_{2,1,2}$ satisfies *three* distinct symmetries, modulo $I_{3,2}$.

Identity 4.3.30. *The integral $I_{2,1,2}$ satisfies the following three basic symmetries modulo $I_{3,2}$.*

$$I_{2,1,2}(ab(cdef)) \overset{I_{3,2}}{=} I_{2,1,2}(ab(fedc)) \tag{4.3.17}$$

$$I_{2,1,2}(ab(cd)(ef)) \overset{I_{3,2}}{=} I_{2,1,2}(ab(dc)(fe)) \tag{4.3.18}$$

$$I_{2,1,2}((ab)cdef) \overset{I_{3,2}}{=} I_{2,1,2}((ba)cdef) \tag{4.3.19}$$

Remark 4.3.31. Since even the number of symmetries differs from the integrals $I_{3,1,1}$ and $I_{2,2,1}$, we certainly cannot write $I_{2,1,2}$ as a single $I_{3,1,1}$ term, or as a single $I_{2,2,1}$ term.

Then $I_{2,1,2}$ satisfies its own type of 4-term identity.

Identity 4.3.32. *$I_{2,1,2}$ satisfies the following 4-term identity modulo $I_{3,2}$.*

$$\operatorname{Alt}_{\{\,d,f\,\}} \operatorname{Cyc}_{\{\,e,f\,\}} I_{2,1,2}(abcdef) \overset{I_{3,2}}{=} 0\,. \tag{4.3.20}$$

Repeated applications of `LatticeReduce` find no 6-term identities. The next identity is then an 8-term identity.

Identity 4.3.33. *$I_{2,1,2}$ satisfies the following 8-term identity modulo $I_{3,2}$*

$$\operatorname{Alt}_{\{\,b,d\,\}} \operatorname{Cyc}_{(ae)(cf)} \operatorname{Cyc}_{(ac)(ef)} I_{2,1,2}(abcdef) \overset{I_{3,2}}{=} 0\,. \tag{4.3.21}$$

The final relation that we need to fully describe the relations of $I_{2,1,2}$ is a 10-term relation. On top of all the previous relations, only one instance of the 10-term relation is required.

Identity 4.3.34. *$I_{2,1,2}$ satisfies the following 10-term identity modulo $I_{3,2}$*

$$\mathrm{Cyc}_{\{a,c,d,e,f\}}\,\mathrm{Cyc}_{\{e,f\}}\,I_{2,1,2}(abcd(ef)) \overset{I_{3,2}}{=} 0 \tag{4.3.22}$$

4.3.6.1 Rank and bases of $I_{2,1,2}$ relations modulo $I_{3,2}$

By considering the relations arising under all permutations of the arguments $abcdef$, we obtain the following table, which counts the number of linearly independent relations arising from each initial relation.

$I_{2,1,2}$ relation	Number of terms	Rank of relations
Equation 4.3.17	2	360
Equation 4.3.18	2	360
Equation 4.3.19	2	360
Equation 4.3.20	4	240
Equation 4.3.21	8	90
Equation 4.3.22	10	138
Overall rank		687

We can take any of the following choices to obtain a 'minimal' basis for the $I_{2,1,2}$ relations, modulo $I_{3,2}$.

$I_{2,1,2}$ relation	Number of terms	Bases	
Equation 4.3.17	2	✓	✓
Equation 4.3.18	2	✓	
Equation 4.3.19	2	✓	✓
Equation 4.3.20	4		✓
Equation 4.3.21	8	✓	✓
Equation 4.3.22	10	✓	✓

4.3.7 Identities for $I_{1,2,2}$ modulo $I_{3,2}$

At depth 3, the final integral we need to consider is $I_{1,2,2}$. At first glance, this integral appear to be even more complicated than $I_{2,2,1}$, requiring a longer final relation to describe the null-space. On the other hand, there are several striking similarities between the relations which do hold, which suggest some other connection between $I_{2,2,1}$ and $I_{1,2,2}$.

The integral $I_{1,2,2}$ satisfies two symmetries.

Identity 4.3.35. *Modulo $I_{3,2}$, the integral $I_{1,2,2}$ satisfies the following symmetries.*

$$I_{1,2,2}(ab(c)d(e)f) \overset{I_{3,2}}{=} I_{1,2,2}(ab(e)d(c)f) \tag{4.3.23}$$

$$I_{1,2,2}((ab)cdef) \overset{I_{3,2}}{=} I_{1,2,2}((ba)cdef) \tag{4.3.24}$$

Remark 4.3.36. The first symmetry Equation 4.3.23, which permutes positions $3 \leftrightarrow 5$, shows that $I_{1,2,2}$ cannot be expressed as a single $I_{2,2,1}$ term, or a single $I_{3,1,1}$ term since the symmetry is structurally different from any symmetry $I_{2,2,1}$ satisfies, or $I_{3,1,1}$ satisfies.

Next, we have a 4-term relation, and a 6 term relation.

Identity 4.3.37. *Modulo $I_{3,2}$, the integral $I_{1,2,2}$ satisfies the following 4-term, and 6-term relations.*

$$\mathrm{Alt}_{(ac)(be)} \mathrm{Alt}_{\{\,d,f\,\}} I_{1,2,2}(abc(d)e(f)) \overset{I_{3,2}}{=} 0 \tag{4.3.25}$$

$$\mathrm{Alt}_{\{\,e,f\,\}} \mathrm{Cyc}_{\{\,c,d,e\,\}} I_{1,2,2}(ab(cde)f) \overset{I_{3,2}}{=} 0\,. \tag{4.3.26}$$

Despite searching, no identity analogous to the unstructured 6-term relation for $I_{2,2,1}$ has turned up. The next identities are therefore 8-term relations.

Identity 4.3.38. *Modulo $I_{3,2}$, the integral $I_{1,2,2}$ satisfies the following 8-term relations.*

$$\mathrm{Cyc}_{(bc)(de)} \mathrm{Cyc}_{(bd)(ce)} \mathrm{Alt}_{\{\,a,f\,\}} I_{1,2,2}((a)bcde(f)) \overset{I_{3,2}}{=} 0 \tag{4.3.27}$$

$$\mathrm{Alt}_{\{\,a,d\,\}} \mathrm{Cyc}_{(bf)(ce)} \mathrm{Cyc}_{(bc)(df)} I_{1,2,2}(a(bc)(d)e(f)) \overset{I_{3,2}}{=} \,. \tag{4.3.28}$$

No version of the unstructured 10-term relation for $I_{2,2,1}$ has turned up yet. However, we do have a 15-term relation, which also occurs by symmetrising the building block of the 6-term relation Equation 4.3.26 differently.

Identity 4.3.39. *Moduo $I_{3,2}$, the integral $I_{1,2,2}$ satisfies the following 15-term relation.*

$$\mathrm{Cyc}_{\{\,b,c,d,e,f\,\}} \mathrm{Cyc}_{\{\,c,d,e\,\}} I_{1,2,2}(ab(cde)f) \overset{I_{3,2}}{=} 0\,. \tag{4.3.29}$$

Currently, in order to fully describe the $I_{1,2,2}$ relations, we can invoke an unstructured 12-term relation, as follows. Since the relation is unstructured, it is almost too powerful – it generates 630 linearly independent relations. Moreover, since it is necessary to describe the relations, it almost forces there to be only one choice of basis for the $I_{1,2,2}$ relations.

Identity 4.3.40. *Modulo $I_{3,2}$, the integral $I_{1,2,2}$ satisfies the followнig 12 term relation.*

$$\begin{aligned} I_{1,2,2}([abedfc] - [abfdce] - [adcbef] + [adecfb] + [adfbec] - [fceabd] + \\ + [fceadb] - [fcebad] + [fcedab] - [fedbac] - [fedcab] + [fedcba]) \overset{I_{3,2}}{=} 0 \end{aligned} \tag{4.3.30}$$

Remark 4.3.41. I do not yet have a clear explanation why there is such a similarity between the $I_{1,2,2}$ relations, and the $I_{2,2,1}$ relations. Certainly, we know that there is no way to write $I_{1,2,2}$ as a single $I_{2,2,1}$ because these integrals exhibit different symmetries.

Even if some short combination of $I_{2,2,1}$'s can be written as a short combination of $I_{1,1,2}$, it would seem some level of good fortune is still necessary to re-write the $I_{1,1,2}$ relations directly to the corresponding $I_{2,2,1}$ relations.

4.3.7.1 Rank and bases of $I_{1,2,2}$ relations modulo $I_{3,2}$

By considering the relations arising under all permutations of the arguments $abcdef$, we obtain the following table, which counts the number of linearly independent relations arising from each initial relation.

$I_{1,2,2}$ relation	Number of terms	Rank of relations
Equation 4.3.23	2	360
Equation 4.3.24	2	360
Equation 4.3.25	4	180
Equation 4.3.26	6	210
Equation 4.3.27	8	90
Equation 4.3.28	8	90
Equation 4.3.29	15	144
Equation 4.3.30	12	630
Overall rank		687

We can take any of the following choices to obtain a 'minimal' basis for the $I_{1,2,2}$ relations, modulo $I_{3,2}$.

$I_{1,2,2}$ relation	Number of terms	Bases
Equation 4.3.23	2	
Equation 4.3.24	2	
Equation 4.3.25	4	
Equation 4.3.26	6	
Equation 4.3.27	8	
Equation 4.3.28	8	
Equation 4.3.29	15	✓
Equation 4.3.30	12	✓

4.4 Higher depth, more arguments, more structure

As we will see in the following chapter, Chapter 5, every integral of weight 5 can be reduced to integrals of depth ≤ 3. So, *in principle*, we do not have to analyse separately the depth 4 integrals $I_{2,1,1,1}$, $I_{1,2,1,1}$, $I_{1,1,2,1}$ or $I_{1,1,1,2}$. Nor do we have to separately analyse the depth 5 integral $I_{1,1,1,1,1}$. Of course, since the reduction to depth ≤ 3 is complicated, trying to read off any relations for these integrals is not an easy task.

On the other hand, fully analysing the symmetries and relations between each of these integrals is computationally much more intensive than the depth 3 cases. For this reason, I have not undertaken a full analysis. I will however indicate a few avenues of investigation.

4.4.1 Reduction of $I_{2,1,1,1}$

At weight 5 we have a kind of analogue of Gangl's result [Gan16] that $I_{2,1,1}$ can be expressed as a sum of 36 terms of the form $\pm\frac{1}{2}I_{3,1}(abcde)$.

Identity 4.4.1. *At weight 5, the integral $I_{2,1,1,1}$ can be expressed, modulo δ, as a sum of 436 terms of the form $\pm I_{3,1,1}(abcdef)$.*

4.4.2 Symmetries and relations for $I_{1,1,1,1,1}$

Modulo δ, the integral $I_{1,1,1,1,1}$ already satisfies a large number of functional equations. Curiously all of the identities which hold modulo δ appear to hold already modulo $\sqcup\!\sqcup$, perhaps because the difference in depth between Li_5 and $I_{1,1,1,1,1}$ is *too* great. Therefore one really should look modulo $I_{3,2}$ to try to find more interesting relations. Unfortunately, the search for relations mod $I_{3,2}$ has, so far, been too computationally intensive to produce any results. Below we will give a selection of identities that $I_{1,1,1,1,1}$ does satisfy.

Identity 4.4.2. *Modulo $\sqcup\!\sqcup$, $I_{1,1,1,1,1}$ satisfies the following two symmetries*

$$I_{1,1,1,1,1}(a(bc)defgh) \overset{\sqcup\!\sqcup}{=} -I_{1,1,1,1,1}(a(cb)defgh)$$
$$I_{1,1,1,1,1}(abc(defgh)) \overset{\sqcup\!\sqcup}{=} I_{1,1,1,1,1}(abc(hgfed))\,.$$

In terms of the arguments v, w, x, y, z, these symmetries say the following

$$I_{1,1,1,1,1}(v,w,x,y,z) \overset{\sqcup\!\sqcup}{=} I_{1,1,1,1,1}(1-v,1-w,1-x,1-y,1-z) \tag{4.4.1}$$
$$I_{1,1,1,1,1}(v,w,x,y,z) \overset{\sqcup\!\sqcup}{=} I_{1,1,1,1,1}(z,y,x,w,v)\,. \tag{4.4.2}$$

Combining Equation 4.4.1 and Equation 4.4.2, we obtain

$$I_{1,1,1,1,1}(v,w,x,y,z) \overset{\sqcup\!\sqcup}{=} -I_{1,1,1,1,1}(1-z,1-y,1-x,1-w,1-v)\,. \tag{4.4.3}$$

This is an example of the limiting case $p \to \infty$ of the Hölder convolution of multiple polylogarithms. See Equation 7.1 in [BBBL01], or Section 1.5.1 in [Rho12]. In fact, Equation 4.4.3 holds on the level of the symbol, and indeed exactly. Equation 4.4.2 fits in the narrative as a higher depth instance of Proposition 4.2.5 and Proposition 4.3.15.

We also have, for example, a 5-term relation where one variable is shuffled through the argument string

Identity 4.4.3. *Modulo $\sqcup\!\sqcup$, $I_{1,1,1,1,1}$ satisfies the following identity*

$$I_{1,1,1,1,1}(v \sqcup\!\sqcup \{\, w,x,y,z \,\}) \overset{\sqcup\!\sqcup}{=} 0\,.$$

Or in full

$$I_{1,1,1,1,1}(v,w,x,y,z) + I_{1,1,1,1,1}(w,v,x,y,z) + I_{1,1,1,1,1}(w,x,v,y,z) + \\ + I_{1,1,1,1,1}(w,x,y,v,z) + I_{1,1,1,1,1}(w,x,y,z,v) \overset{ш}{=} 0 \,. \quad (4.4.4)$$

Of course, Equation 4.4.4 is nothing but the simple fact that using the shuffle product of iterated integrals

$$I_1(v) I_{1,1,1,1}(w,x,y,z) = I_{1,1,1,1,1}(v,w,x,y,z) + I_{1,1,1,1,1}(w,v,x,y,z) + \\ + I_{1,1,1,1,1}(w,x,v,y,z) + I_{1,1,1,1,1}(w,x,y,v,z) + I_{1,1,1,1,1}(w,x,y,z,v) \,.$$

There are still plenty of other identities for $I_{1,1,1,1,1}$ modulo δ left to investigate. But all of them are in some sense too 'simple': they do not involve Li_5 terms. More interesting would be to find identities holding modulo $I_{3,2}$ in the hope that some identities genuinely involve Li_5 and/or $I_{3,2}$ terms. One would also hope that some extra symmetries, or short functional equations, for $I_{1,1,1,1,1}$ hold modulo $I_{3,2}$.

4.4.3 More arguments

As explained at the start of Section 4.1.2, the idea to use coupled cross-ratio arguments comes from Gangl's success with these type of arguments at weight 4, and from their position as natural coordinates on the moduli space $\mathfrak{M}_{0,n}$. One factor for this success is due to the fact that, modulo δ, the integrals look like sums of the form $\sum_i \{\alpha_i\}_2 \wedge \{\beta_i\}_2$. Cross-ratio arguments describe the 5-term relation for Li_2, so fit well with finding relations for weight 4 iterated integrals.

At weight 5, modulo δ, the integrals look like sums of the form $\sum_i \{\alpha_i\}_2 \wedge \{\beta_i\}_3$. For example

$$I_{4,1}(x,y) \overset{\delta}{=} -\{x\}_2 \wedge \{y\}_3 + \{x\}_3 \wedge \{y\}_2 \,.$$

This can be calculated directly using the PolylogTools package [PT] in Mathematica. A calculation by hand, in the manner of Section 3.4.2 is possible (see Proposition 7.5.1), but takes more work than that case $I_{3,1}$ handled there in Example 3.4.12.

The form of weight 5 iterated integrals, modulo δ, suggests that Li_2 and Li_3 arguments would be a sensible choice. Goncharov's triple ratio for Li_3 (see Section 3.2.2) is potentially a good analogue for the Li_2 cross-ratio. Some kind of coupled cross-ratio/triple-ratio arguments could provide an even better source of arguments for identities and relations between weight 5 MPL's.

4.4.4 More structure using representation theory

The identities presented above have a very ad-hoc appearance. They were found entirely using computer linear algebra to determine all possible relations between integrals $I_{n_1,n_2}(\sigma \cdot abcde)$ (modulo ш, modulo δ, modulo $I_{3,2}$), with no real possibility to direct the computer towards structured or aesthetically pleasing identities. In those cases where the identities do not have much structure (e.g.

Identity 4.3.8, and the identities $I_{3,1,1}$ modulo $I_{3,2}$), additional work should be done to find a more structured description of these identities.

In the case where the identities are already highly structured, it should be possible to identify a deeper, theoretical basis for the structure. Specifically, these identities should have a representation theoretic basis since we have an S_{k+3} action on $I_{n_1,\dots,n_k}(abcd_1,\dots,d_k)$. For example, identities like Equation 4.3.20, Equation 4.3.21 and Equation 4.3.22 have a form already reminiscent of, and closely connected to, the representation theory of the symmetric group S_n (every representation of S_n is built up as $\bigwedge^k S^\ell V$, from wedge powers of symmetric powers of some vector space). Furthermore, it has been suggested that the $I_{3,2}$ and Li_5 terms in such identities (e.g. Identity 4.3.14) could have an interpretation as some kind of projection operators on the initial representation.

Chapter 5

Dan's reduction procedure, and a reduction of $I_{1,1,1,1,1}$

In this chapter we will give an account of Dan's reduction method [Dan11] for reducing $I_{1,1,\ldots,1}$ to a sum of integrals of lower depth. We will provide a detailed explanation of the method Dan describes (Section 5.1), including providing the missing proofs for all of Dan's claims. We start off first by giving an overview (Section 5.1.1) of the method itself, then explain Dan's algebraic setup for a space $\mathcal{H}_n(E)$ of multiple polylogarithms (Section 5.1.2), before working through the steps of the method in detail (Section 5.1.3 onwards).

Ultimately this will allow us to provide a corrected version of the Dan's reduction of $I_{1,1,1,1}$ to $I_{3,1}$'s and I_4's (Theorem 5.2.1). Given this, we can use the symbol to compare with Dan's earlier reduction of $I_{1,1,1,1}$ (Theorem 5.2.5, with small a correction by Gangl), and determine the nature of the resulting functional equation of $I_{3,1}$ (Section 5.2.2).

Next, we will apply the method to $I_{1,1,1,1,1}$ at weight 5 (Section 5.3) to produce a reduction to depth ≤ 3 integrals first (Identity 5.3.1) and then to $I_{3,1,1}$, $I_{3,2}$ and I_5, modulo products (Section 5.3.2). Finally we will see how to reduce $I_{3,1,1}$ to $I_{3,2}$, modulo δ (Identity 5.3.5), and indicate how this allows us to reduce $I_{1,1,1,1,1}$ to $I_{3,2}$'s only, modulo δ, (Theorem 5.3.8).

5.1 Dan's reduction method

In [Dan11], Dan gives a systematic method for reducing iterated integrals in n variables to a combination of iterated integrals in $n-2$ variables. This then has the effect of reducing a depth n iterated integral to a sum of depth $n-2$ iterated integrals, so the number of 'slots' for arguments decreases by 2.

The original papers are written in French, are currently unpublished, and provide limited explanation of the steps. Moreover, they contain mistakes in the final calculations. The mistakes, at least in the second paper, do not appear to be the result of simple typos in the final answer. This situation warrants a detailed investigation to determine the correctness of the method. Fortunately the reduction method itself is correct, so by implementing it in Mathematica [MA] I can produce a corrected version of Dan's result. The result I produce is close enough to Dan's (in number of terms, sizes of coefficients, agreement of argument cross-ratios) to make me believe that this was the version he intended to write down. However, it is still not clear exactly where Dan could have made a mistake, and it does not warrant the effort needed to find it.

The goal of this section is to provide an account of the reduction method in these papers, and furnish explanations and proofs for all the steps of the method.

5.1.1 Overview of the reduction method

Firstly, we will give an overview of how the reduction method works. This will allow the reader to have a broad overview of the steps in the method, and not get hung up on the details initially.

Set-up: Introduce (Definition 5.1.4), a slight generalisation

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}) \rightsquigarrow [a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}] \,,$$

of the hyperlogarithm/multiple logarithm/iterated integral $I(x_0; x_1, \ldots, x_m; x_{m+1})$, to be defined using the differential form

$$\omega(a_i, x) \coloneqq \frac{(a_i - x)}{(t - a_i)(t - x)} \, \mathrm{d}t \,.$$

This reduces to the usual hyperlogarithm when $x = \infty$.

Swap out x: Show that the hyperlogarithms obtained by swapping out one of the a_i's with the new parameter x, namely

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}] + [a_0 \mid a_1, \ldots, a_{i-1}, x, a_{i+1}, \ldots, a_n \mathbin{/\!/} a_i \mid a_{n+1}] \,,$$

can be reduced to a sum in $\leq n - 2$ variables (Proposition 5.1.18). This is done with the A and B operators (Definition 5.1.9, Definition 5.1.11), and packaged into the D operator (Definition 5.1.19).

Build a transposition of a_i: Do this three times, to swap a_i out, then a_j out, then x out. This gives a transposition

$$[a_0 \mid a_1, \ldots, a_i, \ldots, a_j, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}] + [a_0 \mid a_1, \ldots, a_j, \ldots, a_i, \ldots, a_n \mathbin{/\!/} a_i \mid a_{n+1}] \,,$$

of the a_i's as a sum in $\leq n - 2$ variables (Proposition 5.1.20).

Apply to $a_1 a_2 \sqcup\!\sqcup\, a_3 \ldots a_n$: Each term in this product can be converted back to $a_1 \ldots a_n$, by some suitable permutation. The previous step allows us to write this as a sum in $\leq n - 2$ variables. (Theorem 5.1.23)

Do this in a structured way: Write down the terms in the following manner

$$\begin{aligned} a_1 a_2 \sqcup a_3 \dots a_n = A_{1,2} + & \\ & + A_{1,3} + A_{2,3} + \\ & + A_{1,4} + A_{2,4} + A_{3,4} + \\ & + A_{1,5} + A_{2,5} + A_{3,5} + A_{4,5} + \cdots , \end{aligned}$$

where $A_{i,j}$ has a_1 in position i, and a_2 in position j. Each $A_{i,j} + A_{i+1,j}$ is a transposition, so can be written as a sum in $\leq n-2$ variables. This leaves $A_{1,2} + A_{1,4} + A_{1,6} + \cdots$. (Lemma 5.1.28)

Finish: Use that $A_{1,2m} = (A_{1,2m} - A_{1,2m-1}) + (A_{1,2m-1} - A_{1,2m-2}) + A_{1,2m-2}$, to replace $A_{1,2m}$ with $A_{1,2m-2}$ and some transpositions that are a sum in $\leq n-2$ variables. Push this all the way down to $A_{1,2}$ (Lemma 5.1.29), and so write $\lfloor n/2 \rfloor A_{1,2}$ as a sum in $\leq n-2$ variables (Theorem 5.1.36).

5.1.2 The space of multiple polylogarithms $\mathcal{H}_n(E)$

Dan explains a generalisation for the construction of the Bloch groups $\mathcal{B}_n(E)$ described in Section 3.2.3 to provide an algebraic description $\mathcal{H}_n(E)$ of the multiple polylogarithms over a field E. Here we briefly outline this construction, so the symbol $\mathcal{H}_n(E)$ is meaningful below.

Write E^{n+2}_* for the following subset of $(n+2)$-tules

$$E^{n+2}_* \coloneqq \{ \, (a_0, \dots, a_{n+1}) \mid a_0 \neq a_1 \text{ and } a_n \neq a_{n+1} \, \} ,$$

which are meant to represent (convergent) iterated integrals.

The iterated integrals $I(x_0; x_1, \dots, x_n; x_{n+1})$ from Section 1.1.3 are invariant under affine transformations $x_i \mapsto a x_i + b$. So consider the quotient

$$E^{n+2}_* / (E^* \times E)$$

where $(\alpha, \beta) \in E^* \times E$ acts as the affine transformations $a_i \mapsto \alpha a_i + \beta$. Write $\mathcal{A}_n(E)$ for the $\mathbb{Q}$-vector space generated by the symbols $[a_0 \mid a_1, \dots, a_n \mid a_{n+1}]$ for $(a_0, \dots, a_{n+1}) \in E^{n+2}_* / (E^* \times E)$.

The graded vector space

$$\mathcal{A}(E) \coloneqq \bigoplus_{n \geq 0} \mathcal{A}_n(E)$$

admits a bialgebra structure. The multiplication is given by the shuffle product (compare with the shuffle product property of Property 1.1.13), as follows

$$\begin{aligned} [a_0 \mid a_1, \dots, a_k \mid a_{k+\ell+1}] \cdot [a_0 \mid a_{k+1}, \dots, a_{k+1} \mid a_{k+\ell+1}] &= [a_0 \mid a_1 \cdots a_k \sqcup a_{k+1} \cdots a_{k+\ell} \mid a_{k+\ell+1}] \\ &= \sum_{\sigma \in S_{k,\ell}} [a_0 \mid a_{\sigma(1)}, \dots, a_{\sigma(k+k)} \mid a_{k+\ell+1}] \, . \end{aligned}$$

Here $S_{k,\ell}$ is the set of (k,ℓ)-shuffles, see Definition 1.1.15. The coproduct is given by Theorem 1.2.1.

The Lie coalgebra $\mathcal{B}^{\mathcal{H}}(E) = \mathcal{A}(E)/(\mathcal{A}_{>0} \cdot \mathcal{A}_{>0})$ of irreducibles admits a co-derivation

$$\delta = \bigoplus_n \left(\delta_n \colon \mathcal{B}^{\mathcal{H}}(E) \to \mathcal{B}^{\mathcal{H}}(E) \otimes \mathcal{B}^{\mathcal{H}}(e)\right) .$$

This will be used to inductively define the vector space of multiple polylogarithm relations $\mathcal{R}^{\mathcal{H}}_n(E) \subset \mathcal{B}^{\mathcal{H}}_n(E)$. We will then set $\mathcal{H}(E) \coloneqq \mathcal{B}^{\mathcal{H}}_n(E)/\mathcal{R}_n(E)$ to be the space of multiple polylogarithms, and write $[a_0 \mid a_1, \ldots, a_n \mid a_{n+1}]$ for the image of the same element in $\mathcal{B}^{\mathcal{H}}(E)$ modulo the relations $\mathcal{R}^{\mathcal{H}}_n(E)$.

The vector space of 1-dimensional relations is generated by the following elements

$$\mathcal{R}^{\mathcal{H}}_1(E) \coloneqq \langle [a \mid z \mid b] + [b \mid z \mid c] = [a \mid z \mid c] \mid z, a, b, c \in E \text{ with } z \neq a, b, c \rangle .$$

Write $\mathcal{K}_n(E)$ for the kernel of the map

$$(\mathrm{pr} \otimes \mathrm{pr}) \circ \delta_n \colon \mathcal{B}^{\mathcal{H}}_n(E) \to (\mathcal{H}(E) \otimes \mathcal{H}(E))_n ,$$

where $\mathrm{pr} \colon \mathcal{B}^{\mathcal{H}}_k(E) \to \mathcal{H}_k(E)$ is already defined for $k < n$.

Definition 5.1.1 (Space of relations $\mathcal{R}^{\mathcal{H}}_n(E)$)**.** The space of multiple polylogarithm relations is generated by the following elements

$$\mathcal{R}^{\mathcal{H}}_n(E) \coloneqq \{ \, \alpha(1) - \alpha(0) \mid \alpha \in \mathcal{K}_n(E(t)) \, \}$$

The map $(\mathrm{pr} \otimes \mathrm{pr}) \circ \delta_n$ factors through $\mathcal{R}^{\mathcal{H}}_n(E)$, to give a map

$$\delta_n \colon \mathcal{H}_n(E) \to (\mathcal{H}(E) \otimes \mathcal{H}(E))_n .$$

This gives $\mathcal{H}(E)$ the structure of a graded Lie coalgebra.

Remark 5.1.2. One can think of $\mathcal{H}_n(E)$ as the space of weight n multiple polylogarithms (or iterated integrals), taken modulo products.

5.1.3 Definition of the generalised hyperlogarithm

Definition 5.1.3. The unique differential form $\omega(a_i, x)$ of degree 1, holomorphic on $\mathbb{P}^1(\mathbb{C}) \setminus \{ \, a_i, x \, \}$ which is 0 if $a_i = x$, and otherwise has a pole of order 1 and residue $+1$ at a_i and a pole of order 1 and residue -1 at x is

$$\omega(a_i, x) \coloneqq \frac{(a_i - x)}{(t - a_i)(t - x)} \, \mathrm{d}t \, .$$

The correct differential form to take when $x = \infty$ is

$$\omega(a_i, \infty) \coloneqq \frac{\mathrm{d}t}{t - a_i} \, ,$$

since this agrees with $\omega(1/a_i, 0)(s)$ under the change of variables $s = 1/t$, sending $\infty \mapsto 0$ and $a_i \mapsto 1/a_i$.

Definition 5.1.4 (Generalised hyperlogarithm)**.** Let $a_i, x \in \mathbb{P}^1(\mathbb{C})$, such that $a_0 \neq a_1$, $a_0 \neq x$, $a_n \neq a_{n+1}$ and $x \neq a_{n+1}$. Then the *generalised hyperlogarithm* $H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1})$ is defined by the following iterated integral

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}) \coloneqq \int_{a_0}^{a_{n+1}} \omega(a_1, x) \circ \omega(a_2, x) \circ \cdots \circ \omega(a_n, x)\,.$$

This should be compared with the definition of Chen's iterated integrals in Definition 1.1.10. Recall from Section 3.1.1 Goncharov's remarks [Gon98; Gon01] that $I(x_0; x_1, \ldots, x_m; x_{m+1})$ are sometimes called hyperlogarithms or multiple logarithms. The relationship between this generalised hyperlogarithm, and the ordinary hyperlogarithm is straightforward.

Proposition 5.1.5. *If $x = \infty$ then*

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} \infty \mid a_{n+1}) = I(a_0; a_1, \ldots, a_n; a_{n+1})\,.$$

Otherwise

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}) = I((a_0 - x)^{-1}; (a_1 - x)^{-1}, \ldots, (a_n - x)^{-1}; (a_{n+1} - x)^{-1})\,.$$

Proof. If $x = \infty$, then the differential form $\omega(a_i, x)$ reduces to the usual form $\frac{\mathrm{d}t}{t - a_i}$ appearing in the definition of the hyperlogarithm.

Otherwise, change variables via $t' = 1/(t - x)$, which sends $x \mapsto \infty$, and $a_i \mapsto 1/(a_i - x)$. We have that $t = \frac{1}{t'} + x$, so that

$$\begin{aligned}
\omega(a_i, x)(t) &= \frac{(a_i - x)}{(t - a_i)(t - x)}\,\mathrm{d}t \\
&= \frac{a_i - x}{(\frac{1}{t'} + x - a_i)(\frac{1}{t'} + x - x)} \frac{-1}{t'^2}\,\mathrm{d}t' \\
&= \frac{1}{t' - \frac{1}{a_i - x}}\,\mathrm{d}t' \\
&= \omega((a_i - x)^{-1}, \infty)(t')\,.
\end{aligned}$$

The bounds a_0 and a_{n+1} change to $(a_0 - x)^{-1}$ and $(a_{n+1} - x)^{-1}$ respectively. ☐

We can use the above relation to the usual hyperlogarithm, to give meaning to the symbol $[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$ in the space $\mathcal{H}_n(E)$ of multiple polylogarithms on 'E' , as follows.

Definition 5.1.6. We set

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} \infty \mid a_{n+1}] \coloneqq [a_0 \mid a_1, \ldots, a_n \mid a_{n+1}]\,,$$

and for $x \neq \infty$,

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}] \coloneqq [(a_0 - x)^{-1} \mid (a_1 - x)^{-1}, \ldots, (a_n - x)^{-1} \mid (a_{n+1} - x)^{-1}]\,.$$

Observation 5.1.7. We can write

$$\omega(a_i, x) = \omega(a_i, y) - \omega(x, y)\,.$$

Proposition 5.1.8. *The hyperlogarithm $H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1})$ can be expressed as an alternating sum of hyperlogarithms of the form $H(a_0 \mid \text{—} \mathbin{/\!/} y \mid a_{n+1})$. More precisely, we have*

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}) = \sum_I (-1)^{\#I}\, H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} y \mid a_{n+1})\big|_{a_I = x}\,,$$

where the sum is taken over all $I \subset \{\, 1, 2, \ldots, n \,\}$, and

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} y \mid a_{n+1})\big|_{a_I = x}$$

means replace a_i by x, for positions $i \in I$.

Proof. We can prove this by induction on the depth n. In the case $n = 1$, we explicitly write out both sides. On the left hand side we have $H(a_0 \mid a_1 \mathbin{/\!/} x \mid a_2)$, and on the right hand side we have

$$\sum_I (-1)^{\#I}\, H(a_0 \mid a_1 \mathbin{/\!/} y \mid a_2)\big|_{a_I = x}\,,$$

taken over all $I \subset \{\, 1 \,\}$. That is, over $I = \emptyset, \{\, 1 \,\}$. This gives

$$H(a_0 \mid a_1 \mathbin{/\!/} y \mid a_2) - H(a_0 \mid x \mathbin{/\!/} y \mid a_2)\,,$$

which is equal to

$$\begin{aligned} \int_{a_0}^{a_2} \omega(a_1, y) - \omega(x, y) &= \int_{a_0}^{a_2} \omega(a_1, x) \\ &= H(a_0 \mid a_1 \mathbin{/\!/} x \mid a_2)\,, \end{aligned}$$

using Observation 5.1.7.

So suppose the result holds for depth $n - 1$. Then for depth n we have the following. We can sum over $I \subset \{\, 1, \ldots, n \,\}$ by first taking I with $1 \in I$, and then taking I with $1 \notin I$. So

$$\begin{aligned} &\sum_I (-1)^{\#I}\, H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} y \mid a_{n+1})\big|_{a_I = x} = \\ &\qquad \sum_{\substack{I \text{ such that} \\ 1 \in I}} (-1)^{\#I}\, H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} y \mid a_{n+1})\big|_{a_I = x} + \\ &\qquad + \sum_{\substack{I \text{ such that} \\ 1 \notin I}} (-1)^{\#I}\, H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} y \mid a_{n+1})\big|_{a_I = x}\,. \end{aligned}$$

In the first sum we know $1 \in I$, so we can remove 1 from I, replace a_1 with x and insert one minus sign already. Then the sum is over $I' \subset \{\, 2, \ldots, n \,\}$. In the second sum, $1 \notin I$, so the sum is over $I' \subset \{\, 2, \ldots, n \,\}$ already, giving

$$= -\sum_{I'} (-1)^{\#I'}\, H(a_0 \mid x, a_2, \ldots, a_n \mathbin{/\!/} y \mid a_{n+1})\big|_{a'_I = x} +$$

$$+\sum_{I'}(-1)^{\#I'}\ H(a_0 \mid a_1, a_2, \ldots, a_n \mathbin{/\!/} y \mid a_{n+1})|_{a'_I = x}\,.$$

Now recall from Remark 1.1.12 that the iterated integral $H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1})$ can be expanded as follows

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}) = \int_{a_0}^{a_{n+1}} H(a_0 \mid a_1, \ldots, a_{n-1} \mathbin{/\!/} x \mid t)\omega(a_n, x)\,.$$

If we do this with the integrals in the sum above, we obtain

$$\begin{aligned} &= \int_{a_0}^{a_{n+1}} \sum_{I'}(-1)^{\#I'}\ H(a_0 \mid a_1, \ldots, a_{n-1} \mathbin{/\!/} y \mid t)|_{a'_I = x} \circ \omega(x, y) + \\ &\quad \sum_{I'}(-1)^{\#I'}\ H(a_0 \mid a_1, \ldots, a_{n-1} \mathbin{/\!/} y \mid t)|_{a'_I = x} \circ \omega(a_n, y) \end{aligned}$$

Using the induction assumption, this can be written as

$$\begin{aligned} &= \int_{a_0}^{a_{n+1}} H(a_0 \mid a_1, \ldots, a_{n-1} \mathbin{/\!/} x \mid t) \circ -\omega(x, y) + \\ &\quad + H(a_0 \mid a_1, \ldots, a_{n-1} \mathbin{/\!/} x \mid t) \circ \omega(a_n, y) \\ &= \int_{a_0}^{a_{n+1}} H(a_0 \mid a_1, \ldots, a_{n-1} \mathbin{/\!/} x \mid t) \circ (\omega(a_n, y) - \omega(x, y)) \\ &= \int_{a_0}^{a_{n+1}} H(a_0 \mid a_1, \ldots, a_{n-1} \mathbin{/\!/} x \mid t) \circ \omega(a_n, x) \end{aligned}$$

using Observation 5.1.7,

$$= H(a_0 \mid a_1, a_2, \ldots, a_n, \mathbin{/\!/} x \mid a_{n+1})\,.$$

This completes the proof. □

5.1.4 Operators A and B

Here we will introduce the operators A and B which will give us tools to systematically reduce the hyperlogarithms.

Definition 5.1.9 (A operator)**.** Let $1 \le i \le n$ and let I be a subset of $\{ 1, 2, \ldots, n \}$ containing i. Define

$$A([a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid A_{n+1}], i, I)$$

to be the symbol

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$$

where the positions $j \in I$ are replaced by the variable a_i from position i.

Example 5.1.10. We have

$$A([a_0 \mid a_1, a_2, a_3, a_4, a_5, a_6 \mathbin{/\!/} x \mid a_7], 3, \{ 2, 3, 5 \}) = [a_0 \mid a_1, a_3, a_3, a_4, a_3, a_6 \mathbin{/\!/} x \mid a_7]$$

$$A([a, \mid b, c, d, e, f, g \mathbin{/\!/} x \mid h], 4, \{ 2, 3, 4, 6 \}) = [a \mid b, e, e, e, f, e \mathbin{/\!/} x \mid h]\,.$$

Definition 5.1.11 (B operator)**.** Now define

$$B([a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}], i) \coloneqq \sum_I (-1)^{\#I} A([a_0, \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}], i, I)\,,$$

where the sum is taken over all subsets I of the set $\{ 1, 2, \ldots, n \}$ containing i and having cardinality $\#I \geq 2$.

Example 5.1.12. With $i = 2$ and $n = 3$, we would have to sum over the sets $\{ 1, 2 \}, \{ 2, 3 \}, \{ 1, 2, 3 \}$. So we get

$$\begin{aligned} B([a_0 \mid a_1, a_2, a_3 \mathbin{/\!\!/} x \mid a_4], 2) = \; & (-1)^{\#\{ 1,2 \}} A([a_0 \mid a_1, a_2, a_3 \mathbin{/\!\!/} x \mid a_4], 2, \{ 1, 2 \}) \\ & + (-1)^{\#\{ 2,3 \}} A([a_0 \mid a_1, a_2, a_3 \mathbin{/\!\!/} x \mid a_4], 2, \{ 2, 3 \}) \\ & + (-1)^{\#\{ 1,2,3 \}} A([a_0 \mid a_1, a_2, a_3 \mathbin{/\!\!/} x \mid a_4], 2, \{ 1, 2, 3 \}) \\ = \; & [a_0 \mid a_2, a_2, a_3 \mathbin{/\!\!/} x \mid a_4] \\ & + [a_0 \mid a_1, a_2, a_2 \mathbin{/\!\!/} x \mid a_4] \\ & - [a_0 \mid a_2, a_2, a_2 \mathbin{/\!\!/} x \mid a_4] \end{aligned}$$

Dan now says that the considerations from Proposition 5.1.8, applied when $y = a_i$, suggest a relation in $\mathcal{H}_n(E)$. Indeed, setting $y = a_i$ in Proposition 5.1.8 gives

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}) = \sum_I (-1)^{\#I} \, H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1})\big|_{a_I = x} \,.$$

Notice that whenever $i \notin I$, so that a_i is not replaced by x, we obtain an integral like $H(a_0 \mid \ldots, a_i, \ldots \mathbin{/\!\!/} a_i \mid a_{n+1})$ which contains the differential form $\omega(a_i, a_i) = 0$. The resulting integral is therefore 0, and does not contribute to the total. It makes sense, then, to reduce the sum to $I \subset \{ 1, 2, \ldots, n \}$, such that $i \in I$. Moreover, there is only one possible I' with $\#I' = 1$, so we can deal with term separately. We obtain

$$\begin{aligned} &= -H(a_0 \mid a_1, \ldots, a_{i-1}, x, a_i, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1}) + \\ &+ \sum_{I'} (-1)^{\#I'} \, H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1})\big|_{a_{I'} = x} \,, \end{aligned}$$

where the sum is taken over all $I' \subset \{ 1, 2, \ldots, n \}$ such that $i \in I$ and $\#I \geq 2$.

Rearranging this gives

$$\begin{aligned} & H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}) + H(a_0 \mid a_1, \ldots, a_{i-1}, x, a_i, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1}) \\ &= \sum_{I'} (-1)^{\#I'} \, H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1})\big|_{a_I = x} \\ &= \sum_{I'} (-1)^{\#I'} \, H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1})\big|_{a_I = a_i} \,. \end{aligned}$$

The last equality comes from the symmetry under $a_i \leftrightarrow x$ in the first line. From this we obtain the following result.

Lemma 5.1.13. *In $\mathcal{H}_n(E)$ the following the following relation holds*

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}] + [a_0 \mid a_1, \ldots, a_{i-1}, x, a_{i+1}, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1}] \\ = B([a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}], i))\,.$$

Proof. We have the result

$$H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}) + H(a_0 \mid a_1, \ldots, a_{i-1}, x, a_{i+1}, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1}) + \\ - B(H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}), i) = 0$$

on the level of integrals. Taking $a_{n+1} \rightsquigarrow a_0 + t(a_{n+1} - a_0)$, we get

$$\alpha(t) = H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_0 + t(a_{n+1} - a_0)) + \\ + H(a_0 \mid a_1, \ldots, a_{i-1}, x, a_{i+1}, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_0 + t(a_{n+1} - a_0)) + \\ - B(H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_0 + t(a_{n+1} - a_0)), i)\,.$$

Now $\alpha(t) = 0$ on the level of integrals means $\alpha(t) \in \mathcal{K}_n(E(t))$. So we find the following relation $\alpha(1) - \alpha(0) \in \mathcal{R}_n^{\mathcal{H}}(E)$. But this evaluates to

$$\alpha(1) - \alpha(0) = H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}) + H(a_0 \mid a_1, \ldots, a_{i-1}, x, a_{i+1}, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1}) + \\ - B(H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}), i)\,.$$

So we get the result claimed. □

Lemma 5.1.14. *In $\mathcal{H}_n(E)$ we have for $0 \leq s \leq n$, that*

$$[a_0 \mid \{y\}^s, b_{s+1}, b_{s+2}, \ldots, b_n \mathbin{/\!\!/} x \mid a_{n+1}] = (-1)^s [a_0 \mid b_{s+1}, (\{y\}^s \sqcup b_{s+2} \cdots b_n) \mathbin{/\!\!/} x \mid a_{n+1}] \\ = (-1)^s \sum_J C_J\,,$$

where C_j denotes the symbol $[a_0 \mid b_{s+1}, \text{—} \mathbin{/\!\!/} x \mid a_{n+1}]$ with the positions J occupied by y, and the remaining positions by $b_{s+1}, \ldots, b_n$ in that order. In the sum, J runs through subsets of size s of the set $\{\, 2, 3, \ldots, n \,\}$.

Proof. First we see this is trivially true for $s = 0$, since we have

$$[a_0 \mid \{y\}^0, b_{0+1}, b_{0+2}, \ldots, b_n \mathbin{/\!\!/} x \mid a_{n+1}] = [a_0 \mid b_1, b_2, \ldots, b_n \mathbin{/\!\!/} x \mid a_{n+1}]\,,$$

and

$$(-1)^0 [a_0 \mid b_{0+1}, (\{y\}^0 \sqcup b_{0+2} \cdots b_n) \mathbin{/\!\!/} x \mid a_{n+1}] = [a_0 \mid b_{0+1}, (\emptyset \sqcup b_{0+2} \cdots b_n) \mathbin{/\!\!/} x \mid a_{n+1}] \\ = [a_0 \mid b_1, b_2, \ldots, b_n \mathbin{/\!\!/} x \mid a_{n+1}]\,.$$

Now comes the inductive step. Recall the inductive definition of ⧢ from Definition 1.1.15. It says that

$$ax ⧢ by = a(x ⧢ by) + b(ax ⧢ y)\,.$$

So we have that

$$\{y\}^{s+1} ⧢ b_{s+2} \cdots b_n = y(\{y\}^s ⧢ b_{s+2} \cdots b_n) + b_{s+2}(\{y\}^{s+1} ⧢ b_{s+3} \cdots b_n)\,. \tag{5.1.1}$$

We therefore compute that

$$\begin{aligned}
&[a_0 \mid \{y\}^{s+1}, b_{s+2}, b_{s+3}, \cdots, b_n \,/\!\!/\, x \mid a_{n+1}] \\
&= [a_0 \mid \{y\}^s, y, b_{s+2}, b_{s+3}, \cdots, b_n \,/\!\!/\, x \mid a_{n+1}] \\
&= (-1)^s [a_0 \mid y(\{y\}^s ⧢ b_{s+2} \cdots b_n) \,/\!\!/\, x \mid a_{n+1}]\,,
\end{aligned}$$

using the induction assumption for s with $b_{s+1} = y$. Now use the relation in Equation 5.1.1, to say

$$\begin{aligned}
&= (-1)^s [a_0 \mid \{y\}^{s+1} ⧢ (b_{s+2} \cdots b_n) - b_{s+2}(\{y\}^{s+1} ⧢ b_{s+3} \cdots b_n) \,/\!\!/\, x \mid a_{n+1}] \\
&= (-1)^{s+1} [a_0 \mid b_{s+1}(\{y\}^{s+1} ⧢ (b_{s+3} \cdots b_n) \,/\!\!/ \mid a_{n+1}]\,,
\end{aligned}$$

since we work modulo products in $\mathcal{H}_n(E)$.

The equality with $\sum_J C_J$ just comes from writing out the terms of the shuffle product. Each term in the shuffle product $b_{s+1}(\{y\}^s ⧢ b_{s+3} \cdots b_n)$ is uniquely determined by which positions contain y. Since we prepend the result with b_{s+1}, these positions are in the range $\{\, 2, 3, \ldots, n \,\}$, and any subset of these occurs. □

Observation 5.1.15. We can apply this to each term $A(S, i, I)$ in $B(S, i)$ from Lemma 5.1.13, with $y = a_i$ and s as large as possible. Firstly, each term in $B(S, i)$ has at least one variable a_j replaced with a_i, so we have reduced the number of variables per term to $n-1$, at most. Then by shuffling out a_i, we can guarantee that it does not appear in the first position. This means $B(s, i)$ is a sum of hyperlogs $[a_0 \mid — \,/\!\!/\, x \mid a_{n+1}]$, where each contains $\leq n-1$ variables, and such that a_i never appears in the first position.

Lemma 5.1.16. *In $\mathcal{H}_n(E)$, the following relation holds for any generic c, specifically c such that $a_1 \neq c$, and $c \neq x$,*

$$[a_0 \mid a_1, \ldots, a_n \,/\!\!/\, x \mid a_{n+1}] = [c \mid a_1, \ldots, a_n \,/\!\!/\, x \mid a_{n+1}] - [c \mid a_1, \ldots, a_n \,/\!\!/\, x \mid a_0]\,.$$

Proof. This follows from the composition of paths property from Property 1.1.13. Given two paths α, β, it states that

$$\int_{\alpha\beta} \omega_1 \circ \cdots \circ \omega_n = \sum_{i=0}^{n} \int_\alpha \omega_1 \circ \cdots \circ \omega_i \int_\beta \omega_{i+1} \circ \cdots \circ \omega_n\,.$$

Recall that the empty integral $\int_\alpha = 1$. If we work modulo products, only the integrals coming from

$i = 0$, and $i = n$ survive. Therefore we have

$$\int_{\alpha\beta} \omega_1 \circ \cdots \circ \omega_n = \int_\alpha \omega_1 \circ \cdots \circ \omega_n + \int_\beta \omega_1 \circ \cdots \circ \omega_n \,,$$

modulo products.

By choosing such a generic c, all the integrals involved will converge. Then take α to be a path $c \to a_0$ and β a path $a_0 \to a_{n+1}$. Choosing $\omega_i = \omega(a_i, x)$ to be our special differential form, we obtain from the above that

$$H(c \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_0) + H(a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}) = H(c \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}) \,,$$

modulo products. Now view this in $\mathcal{H}_n(E)$, and rearrange to obtain the above identity. □

Since a_i does not appear in the first slot, we may use the above to rewrite the terms of the above sum as

$$[a_0 \mid \cdots \mathbin{/\!\!/} x \mid a_{n+1}] = [a_i \mid \cdots \mathbin{/\!\!/} x \mid a_{n+1}] - [a_i \mid \cdots \mathbin{/\!\!/} x \mid a_0]$$

This breaks the single term with $\leq n-1$ variables into two terms each with $\leq n-2$ variables, since a_0 is avoided in favour of the variable a_i in the first summand, and the variable a_{n+1} is avoided in the second summand.

Example 5.1.17. We have

$$\begin{aligned}
&A([a_0 \mid a_1, a_2, a_3, a_4, a_5 \mathbin{/\!\!/} x \mid a_6], 2, \{ 1, 2 \}) \\
&= [a_0 \mid a_2, a_2, a_3, a_4, a_5 \mathbin{/\!\!/} x \mid a_6] \\
&= (-1)^2 [a_0 \mid a_3, (a_2^2 \sqcup\!\sqcup a_4 a_5) \mathbin{/\!\!/} x \mid a_6] \\
&= \ [a_0 \mid a_3, a_2, a_2, a_4, a_5 \mathbin{/\!\!/} x \mid a_6] + [a_0 \mid a_3, a_2, a_4, a_2, a_5 \mathbin{/\!\!/} x \mid a_6] + \\
&\quad + [a_0 \mid a_3, a_4, a_2, a_2, a_5 \mathbin{/\!\!/} x \mid a_6] + [a_0 \mid a_3, a_2, a_4, a_5, a_2 \mathbin{/\!\!/} x \mid a_6] + \\
&\quad + [a_0 \mid a_3, a_4, a_2, a_5, a_2 \mathbin{/\!\!/} x \mid a_6] + [a_0 \mid a_3, a_4, a_5, a_2, a_2 \mathbin{/\!\!/} x \mid a_6]
\end{aligned}$$

And then each term can be split as indicated above. So the first term would become

$$[a_2 \mid a_3, a_2, a_2, a_4, a_5 \mathbin{/\!\!/} x \mid a_6] - [a_2 \mid a_3, a_2, a_2, a_4, a_5 \mathbin{/\!\!/} x \mid a_0] \,,$$

and similarly for the rest.

This proves the following proposition

Proposition 5.1.18. *We may express*

$$\begin{aligned}
&[a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}] + [a_0 \mid a_1, \ldots, a_{i-1}, x, a_{i+1}, \ldots, a_n \mathbin{/\!\!/} a_i \mid a_{n+1}] \\
&\qquad = B([a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}], i) \,,
\end{aligned}$$

as an explicit sum of hyperlogs in $\leq n-2$ *variables.*

5.1.5 Operator D

Definition 5.1.19. The sum in the above Proposition 5.1.18 will be denoted

$$D([a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}], i)\,.$$

Proposition 5.1.20. *A transposition of two variables can be expressed in terms of three D operations as follows*

$$\begin{aligned}&[a_0 \mid a_i, a_j \mathbin{/\!/} x \mid a_{n+1}] + [a_0 \mid a_j, a_i \mathbin{/\!/} x \mid a_{n+1}] \\ &= D([a_0 \mid a_i, a_j \mathbin{/\!/} x \mid a_{n+1}], i) - D([a_0 \mid x, a_j \mathbin{/\!/} a_i \mid a_{n+1}], j) + \\ &\quad + D([a_0 \mid x, a_i \mathbin{/\!/} a_j \mid a_{n+1}], i)\,.\end{aligned}$$

Proof. This is just a case of writing out the result of the three applications of D. Namely

$$\begin{aligned}&D([a_0 \mid a_i, a_j \mathbin{/\!/} x \mid a_{n+1}], i) - D([a_0 \mid x, a_j \mathbin{/\!/} a_i \mid a_{n+1}], j) + \\ &\quad + D([a_0 \mid x, a_i \mathbin{/\!/} a_j \mid a_{n+1}], i) \\ &= ([a_0 \mid a_i, a_j \mathbin{/\!/} x \mid a_{n+1}] + [a_0 \mid x, a_j \mathbin{/\!/} a_i \mid a_{n+1}]) + \\ &\quad - ([a_0 \mid x, a_j \mathbin{/\!/} a_i \mid a_{n+1}] + [a_0 \mid x, a_i \mathbin{/\!/} a_j \mid a_{n+1}]) + \\ &\quad + ([a_0 \mid x, a_i \mathbin{/\!/} a_j \mid a_{n+1}] + [a_0 \mid a_j, a_i \mathbin{/\!/} x \mid a_{n+1}]) \\ &= [a_0 \mid a_i, a_j \mathbin{/\!/} x \mid a_{n+1}] + [a_0 \mid a_j, a_i \mathbin{/\!/} x \mid a_{n+1}]\,.\end{aligned}$$

□

Corollary 5.1.21. *The combination*

$$[a_0 \mid a_i, a_j \mathbin{/\!/} x \mid a_{n+1}] + [a_0 \mid a_j, a_i \mathbin{/\!/} x \mid a_{n+1}]$$

is an explicit sum of hyperlogs in $\leq n-2$ variables. More generally, for any permutation $\sigma \in S_n$,

$$[a_0 \mid \sigma \cdot (a_1, \ldots, a_n) \mathbin{/\!/} x \mid a_{n+1}] - \operatorname{sgn}(\sigma)[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$$

is an explicit sum of hyperlogs in $\leq n-2$ variables.

Proof. The first claim comes because we know/defined D to be such an explicit sum of hyperlogs in $\leq n-2$ variables. Then by decomposing a permutation as a product of transpositions, we get by induction the result for any permutation σ, as follows. Suppose the claim holds for σ. Let $\tau \in S_n$ be a transposition. Then $\operatorname{sgn}(\tau) = -1$, and for $\tau\sigma$ we have

$$\begin{aligned}&[a_0 \mid \tau\sigma \cdot (a_1, \ldots, a_n) \mathbin{/\!/} x \mid a_{n+1}] - \operatorname{sgn}(\tau\sigma)[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}] \\ &= [a_0 \mid \tau\sigma \cdot (a_1, \ldots, a_n) \mathbin{/\!/} x \mid a_{n+1}] - \operatorname{sgn}(\tau)[a_0 \mid \sigma \cdot (a_1, \ldots, a_n) \mathbin{/\!/} x \mid a_{n+1}]) + \\ &\quad - ([a_0 \mid \sigma \cdot (a_1, \ldots, a_n) \mathbin{/\!/} x \mid a_{n+1}] - \operatorname{sgn}(\sigma)[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}])\,.\end{aligned}$$

Both of these summands is a sum in $\leq n-2$ variables, so the claim holds. □

5.1.6 Reducing a single hyperlog

The above considerations all apply to writing a combination of two hyperlogarithms as a sum of hyperlogs in $\leq n-2$ variables. By carefully considering these combinations, it is possible to write a single hyperlogarithm $[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$ in such a manner.

Proposition 5.1.22. *Let S be the set of $(2, n-2)$ shuffles, which can be considered the as the words from $\{ 1, 2 \} \sqcup \{ 3, \ldots, n \}$. Then*

$$\sum_{\sigma \in S} \operatorname{sgn}(\sigma) = \left\lfloor \frac{n}{2} \right\rfloor$$

Proof. Observe that every permutation in the set of $(2, n-2)$-shuffles, is uniquely determined by the position of 1 and the position of 2. Moreover, 2 must appear after 1 since this is the ordering in the original multiplicand. So each term is described by

$$S^n_{i,j} \coloneqq \{ 3, 4, \ldots, \underbrace{1}_{\text{position } i}, \ldots, \underbrace{2}_{\text{position } j}, \ldots \} \,,$$

where $1 \leq i < j \leq n$.

What is $\operatorname{sgn}(S^n_{i,j})$? To put 2 into position j from its original position 2 requires $j-2$ swaps. Then to put 1 into position i from its original position 1 requires a further $i-1$ swaps. So the total number of swaps is $i+j-3$. We find

$$\operatorname{sgn}(S^n_{i,j}) = \begin{cases} -1 & \text{if } i+j \text{ is even} \\ 1 & \text{if } i+j \text{ is odd.} \end{cases}$$

If we sum all the signs, we obtain

$$\sum_{\sigma \in S} \operatorname{sgn}(\sigma) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} \operatorname{sgn}(S^n_{i,j})$$

Observe that in the inner sum, consecutive terms have opposite signs. At term j, the value $i+j$ has one parity, which means at term $j+1$, the parity of $i+(j+1)$ is different. If there are an even number of terms in the inner sum, then they all cancel in pairs to 0. Otherwise the terms after the first cancel, and we are left with $\operatorname{sgn}(S^n_{i,i+1}) = 1$ since $i+(i+1)$ is odd. The number of terms in the inner sum is $n-(i+1)+1 = n-i$, so this is odd if and only if n and i have different parities.

If $n = 2m$ is even, we obtain:

$$\sum_{i=1}^{n} \sum_{j=i+1}^{n} \operatorname{sgn}(S^n_{i,j}) = \sum_{\substack{i=1 \\ i \text{ odd}}}^{2m} 1 = m = \lfloor n/2 \rfloor \,.$$

And if $n = 2m+1$ is odd, we obtain:

$$\sum_{i=1}^{n} \sum_{j=i+1}^{n} \operatorname{sgn}(S^n_{i,j}) = \sum_{\substack{i=1 \\ i \text{ even}}}^{2m+1} 1 = m = \lfloor n/2 \rfloor \,.$$

This proves the result. ∎

There is enough here now to prove that a depth n hyperlog in $n \geq 3$ variables can be reduced to a sum of hyperlogs in $\leq n-2$ variables. We obtain the following.

Theorem 5.1.23. *For $n \geq 3$, the hyperlog*

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$$

can be expressed as a sum of hyperlogs in $\leq n-2$ variables.

Proof. For each $\sigma \in S$, we have that

$$[a_0 \mid \sigma \cdot (a_1, \ldots, a_n) \mathbin{/\!/} x \mid a_{n+1}] - \operatorname{sgn}(\sigma)[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$$

can be expressed as a sum in $\leq n-2$ variables. Now sum over all such $\sigma \in S$. The left hand terms sum over $\{ 1, 2 \} \sqcup \{ 3, \ldots, n \}$. The right hand terms are all the same, so sum to the multiple $\sum_{\sigma \in S} \operatorname{sgn}(\sigma) = \lfloor n/2 \rfloor$. Therefore we get that

$$[a_0 \mid \{ a_1, a_2 \} \sqcup \{ a_3, \ldots, a_n \} \mathbin{/\!/} x \mid a_{n+1}] - \lfloor n/2 \rfloor \, [a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$$

is a sum of hyperlogarithms in $\leq n-2$ variables.

As we work modulo products the first term here is actually 0 if $n \geq 3$, so this shows that

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$$

is $\frac{1}{\lfloor n/2 \rfloor}$ times a sum of hyperlogs in $\leq n-2$ variables. □

It should be noted, however, that the reduction in this theorem is really only intended as a proof-of-concept. The number of terms generated by relating every permutation in $\{ a_1, a_2 \} \sqcup \{ a_3, \ldots, a_n \}$ back to the permutation $\{ a_1, a_2, a_3, \ldots, a_n \}$ is excessive. Dan provided a more structured approach, working only with transpositions. Some of these ideas are already hinted at in the proof of Proposition 5.1.22.

5.1.7 More structured approach

5.1.7.1 Sructured approach for any n

While the previous section does indeed illustrate a general reduction procedure which can be applied to give correct results, the number of terms generated by decomposing all such shuffles as a sum in $\leq n-2$ variables is large. Dan provides a more structured approach, which we will now explain.

Definition 5.1.24. Define the symbol $A^n_{i,j}$ to be the following

$$A^n_{i,j} \coloneqq [a_0 \mid a_3, a_4, \ldots, \underbrace{a_1}_{\text{position } i}, \ldots, \underbrace{a_2}_{\text{position } j}, \ldots \mathbin{/\!/} x \mid a_{n+1}] \,,$$

where position i is filled with a_1, and position j is filled with a_2. The remaining positions are filled with $a_3, \ldots, a_n$ in this order. (Notice the similarity to $S^n_{i,j}$ from the proof of Proposition 5.1.22, essentially $A^n_{i,j} = [a_0 \mid S^n_{i,j} \mathbin{/\!/} x \mid a_{n+1}]$.)

In the original article, Dan uses the notation $A_{i,j}$, leaving the dependence on n implicit only. For clarity here, and later, I write $A^n_{i,j}$ in order to make the dependence on n as explicit as possible. Similarly we will write R^n where Dan later write R, and c^n where Dan writes c.

Example 5.1.25. With $n = 7$, and $i = 2, j = 5$, we have

$$A^7_{2,5} = [a_0 \mid a_3, \underbrace{a_1}_{\text{position 2}}, a_4, a_5, \underbrace{a_2}_{\text{position 5}}, a_6, a_7 \mathbin{/\!/} x \mid a_8]$$

Lemma 5.1.26. *Consider now the expression $A^n_{i-1,j} + A^n_{i,j}$. This can be expressed as an explicit sum of hyperlogs in $\leq n - 2$ variables. Similarly $A^n_{i,j} + A^n_{i,j+1}$ can be expressed as an explicit sum of hyperlogs in $\leq n - 2$ variables.*

Proof. Going from $A^n_{i-1,j}$ to $A^n_{i,j}$ requires a single transposition swapping positions $i - 1$ and i. Similarly, going from $A^n_{i,j}$ to $A^n_{i,j+1}$ requires a single transposition swapping positions j and $j + 1$. So by Corollary 5.1.21 the result follows. ☐

Definition 5.1.27. Write $R^n(i-1, j \mid i, j)$ for the relation above expressing $A^n_{i-1,j} + A^n_{i,j}$ as a sum in $\leq n - 2$ variables. And write $R^n(i, j \mid i, j + 1)$ for the relation expressing $A^n_{i,j} + A^n_{i,j+1}$ as a sum in $\leq n - 2$ variables.

At this point Dan considers some remarkable sum of R^n's with certain coefficients $c^n(\text{—})$, and claims (without proof) that from this one deduces a reduction formula. I want to motivate this sum in a step-by-step manner, and fill in the missing proofs.

Consider the shuffle product $\{ 1, 2 \} \sqcup\!\sqcup \{ 3, 4, \ldots, n \}$. Each term of this is a word of length n where 1 and 2 occupy certain positions, and the string $3, 4, \ldots, n$ covers the remaining positions in order. Therefore each term of the shuffle product is $A^n_{i,j}$ for some i, j. Moreover, since 1 always occurs at a position before 2, we have $i < j$. Otherwise there is complete freedom to choose i and j between 1 and n. Therefore

$$[a_0 \mid \{ 1, 2 \} \sqcup\!\sqcup \{ 3, 4, \ldots, n \} \mathbin{/\!/} x \mid a_{n+1}] = \sum_{1 \leq i < j \leq n} A^n_{i,j} \,.$$

Now sum in the following order to get

$$\sum_{1 \leq i < j \leq n} A^n_{i,j} = \sum_{j=2}^{n} \sum_{i=1}^{j-1} A^n_{i,j} \,.$$

When j is odd, the inner sum $\sum_{i=1}^{j-1} A^n_{i,j}$ can be written

$$\sum_{\substack{i=1 \\ i \text{ even}}}^{j-1} (A^n_{i-1,j} + A^n_{i,j}) = \sum_{\substack{i=1 \\ i \text{ even}}}^{j-1} R^n(i-1, j \mid i, j) \,.$$

When j is even, the inner sum $\sum_{i=1}^{j-1} A^n_{i,j}$ can be written

$$A_{1,j} + \sum_{\substack{i=3 \\ i \text{ odd}}}^{j-1} (A^n_{i-1,j} + A^n_{i,j}) = A^n_{1,j} + \sum_{\substack{i=3 \\ i \text{ odd}}}^{j-1} R(i-1, j \mid i, j)^n$$

For convenience we want to sum over the full range $i = 2, \ldots, j-1$, including all even and odd indices, but this will introduce spurious extra terms. To fix this, introduce coefficients $c^n(i-1, j, \mid i, j)$ corresponding to the relation $R^n(i-1, j \mid i, j)$. When j is odd we need the even terms to live, so impose $c^n(i-1, j \mid i, j) = 1$ when i even and j odd, and $c^n(i-1, j \mid i, j) = 0$ when i odd and j odd. When j is even, we need the odd terms to live, so impose $c^n(i-1, j \mid i, j) = 1$ when i odd and j even, and $c^n(i-1, j \mid i, j) = 0$ when i even and j even. This can be summarised by saying

$$c^n(i-1, j \mid i, j) = \begin{cases} 1 & \text{if } i-j \text{ odd} \\ 0 & \text{otherwise,} \end{cases}$$

in accordance with Dan's definition. (We write c^n rather than just c because a later extension of c will explicitly depend on n.)

Plugging these into the sum above, we find that

$$[a_0 \mid \{ a_1, a_2 \} \sqcup \{ a_3, a_4, \ldots, a_n \} \mathbin{/\!/} x \mid a_{n+1}] = \sum_{2 \le i < j \le n} c(i-1, j \mid i, j) R^n(i-1, j \mid i, j) + \sum_{\substack{j=2 \\ j \text{ even}}}^{n} A^n_{1,j}$$

Now consider the leftover terms $\sum_{\substack{j=2 \\ j \text{ even}}}^{n} A^n_{1,j}$. Observe that we can write the following equality

$$\begin{aligned} A^n_{1,j} &= (A^n_{1,j} + A_{1,j-1^n}) - (A^n_{1,j-1} + A^n_{1,j-2}) + A^n_{1,j-2} \\ &= R^n(1, j-1 \mid 1, j) - R^n(1, j-2 \mid 1, j-1) + A^n_{1,j-2} \end{aligned}$$

and by iterating,

$$\begin{aligned} &= R^n(1, j-1 \mid 1, j) - R^n(1, j-2 \mid 1, j-1) + \\ &\quad + R^n(1, j-3 \mid 1, j-2) - R^n(1, j-4 \mid 1, j-3) + A^n_{1,j-4} \,. \end{aligned}$$

This means we can eliminate $A^n_{1,j}$ in favour of $A^n_{1,j-2}$ and some relations R^n. By iterating this, we can push this as far as we want, as follows.

Lemma 5.1.28. *For any even $2 \le m \le j-2$, we have*

$$A^n_{1,j} = \sum_{\substack{k=m \\ k \text{ even}}}^{j-2} \left(R^n(1, k+1 \mid 1, k+2) - R^n(1, k \mid 1, k+1) \right) + A^n_{1,m} \,.$$

Proof. Certainly the result is true for $m = j-2$, by the observation preceding this lemma.

Now suppose the result holds for m. Then for $m-2$ we have

$$\begin{aligned} &\sum_{\substack{k=m-2 \\ m \text{ even}}}^{j-2} \left(R^n(1, k+1 \mid 1, k+2) - R^n(1, k \mid 1, k+1) \right) \\ &= \sum_{\substack{k=m \\ m \text{ even}}}^{j-2} \left(R^n(1, k+1 \mid 1, k+2) - R^n(1, k \mid 1, k+1) \right) + \end{aligned}$$

$$+\left(R^n(1,m-1\mid 1,m)-R^n(1,m-2\mid 1,m-1)\right),$$

which by the induction assumption equals

$$\begin{aligned}
&= A^n_{1,j} - A^n_{1,m} + \left(R^n(1,m-1\mid 1,m)-R^n(1,m-2\mid 1,m-1)\right)\\
&= A^n_{1,j} - A^n_{1,m} + \left((A^n_{1,m-1}+A^n_{1,m})-(A^n_{1,m-2}+A^n_{1,m-1})\right)\\
&= A^n_{1,j} - A^n_{1,m-2}\,.
\end{aligned}$$

So the result holds for $m-2$ also. □

In particular, for $m = 2$, we obtain

$$A^n_{1,j} = \sum_{\substack{k=2\\ k \text{ even}}}^{j-2} \left(R^n(1,k+1\mid 1,k+2)-R^n(1,k\mid 1,k+1)\right) + A^n_{1,2}\,,$$

and we can use this to establish the following result.

Lemma 5.1.29. *The sum of the leftover terms is given by*

$$\begin{aligned}
\sum_{\substack{j=2\\ j\ even}}^{n} A^n_{1,j} = \lfloor n/2\rfloor\, A^n_{1,2} &+\\
&+ \sum_{\substack{j=2\\ j\ even}}^{n-2} (\lfloor n/2\rfloor - j/2)\left(R^n(1,j+1\mid 1,j+2)-R^n(1,j\mid 1,j+1)\right)
\end{aligned}$$

Proof. We may use the above result to give an expression for $A^n_{1,j}$, and sum as follows

$$\begin{aligned}
\sum_{\substack{j=2\\ j \text{ even}}}^{n} A_{i,j} &= \sum_{\substack{j=2\\ j \text{ even}}}^{n} \left(A^n_{1,2} + \sum_{\substack{k=2\\ k \text{ even}}}^{j-2} \left(R^n(1,k+1\mid 1,k+2)-R^n(1,k\mid 1,k-1)\right)\right)\\
&= \lfloor n/2\rfloor\, A^n_{1,2} + \sum_{\substack{j=2\\ j \text{ even}}}^{n}\sum_{\substack{k=2\\ k \text{ even}}}^{j-2} \left(R^n(1,k+1\mid 1,k+2)-R^n(1,k\mid 1,k+1)\right).
\end{aligned}$$

Now swap the order of summation, to obtain

$$= \lfloor n/2\rfloor\, A^n_{1,2} + \sum_{\substack{k=2\\ k \text{ even}}}^{n-2}\sum_{\substack{j=k+2\\ j \text{ even}}}^{n} \left(R^n(1,k+1\mid 1,k+2)-R^n(1,k\mid 1,k+1)\right).$$

Since the summand does not depend on the index of the inner sum, we just obtain a multiple of it based on the number of terms summed. In this case we have $\lfloor n/2\rfloor - k/2$ terms, so we get

$$= \lfloor n/2\rfloor\, A^n_{1,2} + \sum_{\substack{k=2\\ k \text{ even}}}^{n-2} (\lfloor n/2\rfloor - k/2)\left(R^n(1,k+1\mid 1,k+2)-R^n(1,k\mid 1,k+1)\right)$$

Finally, change the summation index from k to j to obtain the result. □

Here Dan also wishes to sum over the full range $j = 2,\ldots,n-2$. This is more straightforward to do, since we can break the sum up and reindex it as follows.

$$\sum_{\substack{j=2 \\ j \text{ even}}}^{n-2} (\lfloor n/2 \rfloor - j/2)(R^n(1, j+1 \mid 1, j+2) - R^n(1, j \mid 1, j+1))$$
$$= \sum_{\substack{j=2 \\ j \text{ even}}}^{n-2} (\lfloor n/2 \rfloor - j/2) R^n(1, j+1 \mid 1, j+2) - \sum_{\substack{j=2 \\ j \text{ even}}}^{n-2} (\lfloor n/2 \rfloor - j/2) R^n(1, j \mid 1, j+1) \,.$$

Now put $j \mapsto j-1$ in the first sum. The range chances to $j = 3$ to $n-1$, j odd, giving

$$= \sum_{\substack{j=3 \\ j \text{ odd}}}^{n-1} (\lfloor n/2 \rfloor - (j-1)/2) R^n(1, j \mid 1, j+1) - \sum_{\substack{j=2 \\ j \text{ even}}}^{n-2} (\lfloor n/2 \rfloor - j/2) R^n(1, j \mid 1, j+1) \,.$$

Observe that when j is odd, $(j-1)/2 = \lfloor j/2 \rfloor$. And when j is even, $j/2 = \lfloor j/2 \rfloor$. Both sums can be combined to give

$$= -\sum_{j=2}^{n-1} (-1)^j (\lfloor n/2 \rfloor - \lfloor j/2 \rfloor) R^n(1, j \mid 1, j+1) \,.$$

We can then set

$$c^n(1, j \mid 1, j+1) = (-1)^j (\lfloor n/2 \rfloor - \lfloor j/2 \rfloor) \,,$$

in accordance with Dan. (Writing c^n rather than just c to emphasis the dependence on n.)

Overall, we have

$$\begin{aligned} &[a_0 \mid \{ a_1, a_2 \} \sqcup \{ a_3, a_4, \ldots, a_n \} \mathbin{/\!/} x \mid a_{n+1}] \\ &= \sum_{2 \leq i < j \leq n} c^n(i-1, j \mid i, j) R(i-1, j \mid i, j) + \lfloor n/2 \rfloor \, A^n_{1,2} + \\ &\quad - \sum_{j=2}^{n-1} c^n(1, j \mid 1, j+1) R^n(1, j \mid 1, j+1) \,. \end{aligned}$$

By rearranging this, we therefore obtain the following theorem

Theorem 5.1.30. *The following equality holds*

$$\begin{aligned} \lfloor n/2 \rfloor \, [a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}] = \\ - \sum_{2 \leq i < j \leq n} c^n(i-1, j \mid i, j) R(i-1, j \mid i, j) + \\ + \sum_{2 \leq j \leq n-1} c^n(1, j \mid 1, j+1) R^n(1, j \mid 1, j+1) + \\ + [a_0 \mid \{ a_1, a_2 \} \sqcup \{ a_3, \ldots, a_n \} \mathbin{/\!/} x \mid a_{n+1}] \,. \end{aligned}$$

And in particular for $n \geq 3$,

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}] \,,$$

is explicitly given as a sum of hyperlogs in $\leq n-2$ variables, modulo products.

Corollary 5.1.31. *By setting $x = \infty$, we get an expression for $[a_0 \mid a_1, \ldots, a_n \mid a_{n+1}]$ as a sum of* *hyperlogs in* $\leq n-2$ *variables.*

5.1.7.2 Structured approach for n odd

Dan remarks that when n is odd, one can obtain an even simpler expression for this reduction. This is done as follows.

Lemma 5.1.32. *Let* S *be the set of* $(1, n-1)$ *shuffles, which can be identified with the terms in the shuffle product* $a_1 ⧢ (a_2 \dots a_n)$*. Then*

$$\sum_{\sigma \in S} \operatorname{sgn}(\sigma) = 1\,.$$

Proof. Each term in S is completely determined by the position of a_1. If a_1 is in position j, then it takes $j-1$ swaps to put the permutation into the original order. Hence

$$\sum_{\sigma \in S} \operatorname{sgn}(\sigma) = \sum_{j=1}^{n} (-1)^{j-1}\,.$$

Since $n = 2k+1$ is odd, we can break this up into

$$\begin{aligned} &= \sum_{\substack{j=1 \\ j \text{ even}}} (-1) + \sum_{\substack{j=1 \\ j \text{ odd}}} 1 \\ &= j \cdot (-1) + (j+1) \cdot 1 \\ &= 1\,. \end{aligned}$$

This completes the proof. ☐

Definition 5.1.33. Write

$$A_i^n \coloneqq [a_0 \mid a_2, \dots, a_i, \underbrace{a_1}_{\text{position } i}, a_{i+1}, \dots, a_n \mathbin{/\!/} x \mid a_{n+1}]\,,$$

where position i is filled with a_1, and the remaining positions are filled with $a_2, \dots, a_n$ in this order.

Lemma 5.1.34. *Consider the expression* $A_i^n + A_{i+1}^n$*. This can be expressed as an explicit sum of hyperlogs in* $\leq n-2$ *variables.*

Proof. Observe that $A_i^n + A_{i+1}^n$ is a transposition, obtained by swapping positions i and $i+1$. Since it is a transposition, it can be expressed as a sum in $\leq n-2$ variables using the Corollary 5.1.21 and the D operator. So the result holds. ☐

Definition 5.1.35. Denote by R_i^n the relation expressing $A_i^n + A_{i+1}^n$ as a sum in $\leq n-2$ variables.

Since each term in $[a_0 \mid \{\, a_1 \,\} ⧢ \{\, a_2, \dots, a_n \,\} \mathbin{/\!/} x \mid a_{n+1}]$ is determined by the position of a_1, we obtain

$$[a_0 \mid \{\, a_1 \,\} ⧢ \{\, a_2, \dots, a_n \,\} \mathbin{/\!/} x \mid a_{n+1}] = \sum_{i=1}^{n} A_i^n\,.$$

Since n is odd, we may write this as

$$= A_1^n + \sum_{\substack{i=2 \\ i \text{ even}}}^{n} A_i^n + A_{i+1}^n = A_1^n + \sum_{\substack{i=2 \\ i \text{ even}}}^{n} R_i^n$$
$$= A_1^n + \sum_{j=1}^{\lfloor n/2 \rfloor} R_{2j}^n \,.$$

By rearranging this, we obtain the following theorem.

Theorem 5.1.36. *For odd n, the following equality holds*

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}] =$$
$$[a_0 \mid \{\, a_1 \,\} \sqcup \{\, a_2, \ldots, a_n \,\} \mathbin{/\!\!/} x \mid a_{n+1}] - \sum_{j=1}^{\lfloor n/2 \rfloor} R_{2j}^n \,.$$

And in particular for odd $n \geq 3$,

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}] \,,$$

is explicitly given as a sum of hyperlogs in $\leq n-2$ variables, modulo products.

5.1.8 Reduction of generalised hyperlog to I

When we apply this procedure, we will obtain a number of terms of the form

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}] \,.$$

Ultimately we want to convert these back to the usual iterated integrals $I_{n_1,\ldots,n_k}$. Doing this will give arguments involving cross-ratios as follows.

Firstly, convert this to an ordinary hyperlogarithm, with $x \rightsquigarrow \infty$, by writing

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!\!/} x \mid a_{n+1}] = [(a_0 - x)^{-1} \mid (a_1 - x)^{-1}, \ldots, (a_n - x)^{-1} \mathbin{/\!\!/} \infty \mid (a_{n+1} - x)^{-1}] \,.$$

This ordinary hyperlogarithm is invariant under affine transformation, so apply the translation $t \mapsto t - (a_0 - x)^{-1}$. This sets the lower bound of integral to 0. The other arguments change as follows

$$\frac{1}{a_i - x} \mapsto \frac{1}{a_i - x} - \frac{1}{a_0 - x} = \frac{a_0 - a_i}{(a_i - x)(a_0 - x)} \,.$$

Now apply the scaling $t \mapsto t \frac{(a_{n+1} - x)(a_0 - x)}{a_0 - a_{n+1}}$, which sets the upper bound of the integral to 1. The other arguments change to

$$\frac{a_0 - a_i}{(a_i - x)(a_0 - x)} \mapsto \frac{a_0 - a_i}{(a_i - x)(a_0 - x)} \frac{(a_{n+1} - x)(a_0 - x)}{a_0 - a_{n+1}}$$
$$= \frac{(a_0 - a_i)(a_{n+1} - x)}{(a_i - x)(a_0 - a_{n+1})}$$
$$= \operatorname{cr}(a_{n+1}, a_i, x, a_0) \,.$$

Overall, we find that

$$[a_0 \mid a_1, \ldots, a_n \mathbin{/\!/} x \mid a_{n+1}]$$
$$= [0 \mid \mathrm{cr}(a_{n+1}, a_1, x, a_0), \ldots, \mathrm{cr}(a_{n+1}, a_n, x, a_0) \mid 1] \,.$$

In the Dan reduction procedure, the number of variables is reduced from n to $n-2$ in each integral. This means that at least 2 a_i's will equal a_0 in the terms we apply this to. In this situation the cross-ratio reduces to 0 (or indeed the argument will be identically 0 after the translation step), which has the effect of reducing the depth of the iterated integral by 2 to $n-2$.

5.2 Reduction of $I_{1,1,1,1}$

5.2.1 Procedure when $n = 4$, correcting Dan's reduction of $I_{1,1,1,1}$

In this section we will run this method for $n = 4$, in order to correct the expression Dan gives for $I_{1,1,1,1}(w, x, y, z)$, or more precisely for $I(a; b, c, d, e; f)$. We can obtain the reduction for $I_{1,1,1,1}(w, y, x, z)$ by setting $a = 0$ and $f = 1$.

Firstly, apply Theorem 5.1.30, with $n = 4$ to obtain

$$2[a_0 \mid a_1, a_2, a_3, a_4 \mathbin{/\!/} x \mid a_5]$$
$$= (R^4(1, 2 \mid 1, 3) - R^4(1, 3, \mid 1, 4)) - (R^4(1, 3, \mid 2, 3) - R^4(2, 4 \mid 3, 4)) \,.$$

Let us focus on the term $R^4(1, 2 \mid 1, 3)$ now. This is supposed to be the expression for

$$A^4_{1,2} + A^4_{1,3} = [a_0 \mid a_1, a_2, a_3, a_4 \mathbin{/\!/} x \mid a_5] + [a_0 \mid a_1, a_3, a_2, a_4 \mathbin{/\!/} x \mid a_5] \,,$$

as a sum in $\leq n-2$ variables, using the D operator and Proposition 5.1.20. By this, we have

$$\begin{aligned} A^4_{1,2} + A^4_{1,3} = {} & D([a_0 \mid a_1, a_2, a_3, a_4 \mathbin{/\!/} x \mid a_5], 2) + \\ & - D([a_0 \mid a_1, x, a_3, a_4 \mathbin{/\!/} a_2 \mid a_5], 3) + \\ & + D([a_0 \mid a_1, x, a_2, a_4 \mathbin{/\!/} a_3 \mid a_5], 2) \,. \end{aligned} \tag{5.2.1}$$

Now each D is an explicit sum in $\leq n-2$ variables, using Proposition 5.1.18 and the operator B. Doing this for the first term gives

$$\begin{aligned} D([a_0 \mid a_1, a_2, a_3, a_4 \mathbin{/\!/} x \mid a_5], 2) &= B([a_0 \mid a_1, a_2, a_3, a_4 \mathbin{/\!/} x \mid a_5], 2) \\ &= \sum_I (-1)^{\#I} A([a_0 \mid a_1, a_2, a_3, a_4 \mathbin{/\!/} x \mid a_5], 2, I) \,, \end{aligned}$$

where the sum runs over all $I \subset \{ 1, 2, \ldots, n \}$ containing 2 and having $\#I \geq 2$. In this case the I ranges over the subsets $\{ 1, 2 \}$, $\{ 2, 3 \}$, $\{ 2, 4 \}$, $\{ 1, 2, 3 \}$, $\{ 1, 2, 4 \}$, $\{ 2, 3, 4 \}$ and $\{ 1, 2, 3, 4 \}$. We obtain

$$= [a_0 \mid a_2, a_2, a_3, a_4 \mathbin{/\!\!/} x \mid a_5] + [a_0 \mid a_1, a_2, a_2, a_4 \mathbin{/\!\!/} x \mid a_5] + [a_0 \mid a_1, a_2, a_3, a_2 \mathbin{/\!\!/} x \mid a_5] + \\ - [a_0 \mid a_2, a_2, a_2, a_4 \mathbin{/\!\!/} x \mid a_5] - [a_0 \mid a_2, a_2, a_3, a_2 \mathbin{/\!\!/} x \mid a_5] - [a_0 \mid a_1, a_2, a_2, a_2 \mathbin{/\!\!/} x \mid a_5] + \\ + [a_0 \mid a_2, a_2, a_2, a_2 \mathbin{/\!\!/} x \mid a_5] \,.$$

From here a_2 must be shuffled out of the first position of each term using Lemma 5.1.14. This will let us express each term as the difference of an integral from a_2 to a_0 and from a_2 to a_5, as in Lemma 5.1.16. Doing so gives

$$= \phi(a_0) - \phi(a_5) \,,$$

where

$$\phi(c) = [a_2 \mid a_1, a_2, a_2, a_2 \mathbin{/\!\!/} x \mid c] - [a_2 \mid a_1, a_2, a_2, a_4 \mathbin{/\!\!/} x \mid c] - [a_2 \mid a_1, a_2, a_3, a_2 \mathbin{/\!\!/} x \mid c] + \\ + 3[a_2 \mid a_3, a_2, a_2, a_2 \mathbin{/\!\!/} x \mid c] - [a_2 \mid a_3, a_2, a_2, a_4 \mathbin{/\!\!/} x \mid c] - [a_2 \mid a_3, a_2, a_4, a_2 \mathbin{/\!\!/} x \mid c] + \\ - [a_2 \mid a_3, a_4, a_2, a_2 \mathbin{/\!\!/} x \mid c] - [a_2 \mid a_4, a_2, a_2, a_2 \mathbin{/\!\!/} x \mid c] \,.$$

Now this must be repeated for the other two occurrences of D in Equation 5.2.1, in order to get an expression for $R^4(1, 2 \mid 1, 3)$. Then the whole procedure must be repeated for the remaining 3 relations R^4.

After doing this, we may use the following identities to convert between $I_{1,3}$, and $I_{2,2}$ and $I_{3,1}$

$$I_{2,2}(x, y) \overset{\sqcup\!\sqcup}{=} -I_{1,3}(x, y) - I_{1,3}(y, x) - I_{3,1}(x, y) \\ I_{1,3}(x, y \overset{\sqcup\!\sqcup}{=} I_4(x) - I_{3,1}(x, \tfrac{x}{y}) \,.$$

By converting all terms of the result to $I_{3,1}$ and I_4 we obtain the following theorem.

Theorem 5.2.1 (Correction to Théorème 2 in [Dan11])**.** *As shorthand, write* $abcd \coloneqq \mathrm{cr}(a, b, c, d)$*, and* $abc \coloneqq \mathrm{cr}(a, b, c, \infty)$*. Moreover, write* $[x, y] \coloneqq [x, y]_{3,1} = [0 \mid x, 0, 0, y \mid 1]$ *and* $[x] \coloneqq [x]_4 = [0 \mid x, 0, 0, \mid 1]$*. Then modulo products*

$$[a \mid b, c, d, e \mid f] = \phi(a; b, c, d, e) - \phi(f; b, c, d, e) \,,$$

where

$$2\phi(a; b, c, d, e) \coloneqq \\ [abcd, aecd] - [abcd, dcb] + [abce, bdec] + [abce, cea] - [abce, ecb] + \\ + 2[abd, acd] - 2[abd, aed] - [abd, ebd] + [abe, ace] - [acbd, dbc] + \\ + [acbe, ebc] - 2[acd, bcd] + [ace, bce] - [ace, dce] - [adbe, acbe] + \\ + [adbe, ebd] - [adce, cea] - [adce, ecd] - [ade, abe] + [ade, bde] + \\ - [ade, cde] - [aebd, bdce] - [aecd, dce] - [aed, bed] - 2[bac, bdc] + \\ + [bac, dac] + [bda, acbd] - [bda, aebd] - [bda, bdc] + [bea, acbe] + \tag{5.2.2}$$

$$
\begin{aligned}
&+ [bea, bec] - [cab, cdb] + [cab, ceb] - [cda, aecd] - [cda, cde] + \\
&- [cea, ceb] + [cea, ced] + 2[dab, cab] + [dab, dcb] - 2[dab, eab] + \\
&- [dac, dbc] - [dac, dec] - [dac, eac] + [eab, ecb] - 2[eac, edc] + \\
&\quad + \gamma(a; b, c, d, e) \,.
\end{aligned}
$$

And

$$
\begin{aligned}
\gamma(a; b, c, d, e) \coloneqq {} & [abce] + 5[abd] - 4[abe] + 4[acbd] - 2[acbe] + 2[acd] + 2[ace] + \\
& - 2[adce] + 2[ade] + 2[aecd] + [aed] + 2[bac] + 2[bda] - 4[bea] + \\
& - 2[cab] + 4[cda] + 3[cea] + [dab] + 8[dac] - 3[eab] + 2[eac]
\end{aligned}
$$

is an explicit sum of I_4's of rational functions.

Remark 5.2.2. In the original paper, Dan does not give the I_4 terms explicitly, but says only that such an explicit linear combination exists. Here it is given explicitly for completeness.

This expression has been obtained by implementing Dan's reduction method in Mathematica [MA], and converting to $I_{3,1}$ via the above identities. The final result has been checked using Duhr's PolylogTools package [PT] to confirm the symbol vanishes modulo products. Lastly the TeXutilities package [TU] for Mathematica was used to automatically LaTeX the resulting expression to ensure no typos occured.

Remark 5.2.3. All of the terms in Equation 5.2.2 can in fact be written in the 'coupled cross-ratio' form from Section 4.1.2. For example, in the first term $[abcd, aecd] = [abcd, aecd]_{3,1}$, of Equation 5.2.2, the cross-ratios can be re-written to show that $[abcd, aecd]_{3,1} = [cdab, cdae]_{3,1}$. But now this term can be written using the 'couple cross-ratio' shorthand to give

$$
[abcd, aecd]_{3,1} = I_{3,1}(cdabe) \,.
$$

By reintroducing ∞'s if necessary, the same thing works for all the remaining terms. For example, the second term gives

$$
[abcd, dcb]_{3,1} = I_{3,1}(dcba\infty) \,.
$$

On the level of symbols, this result holds modulo products. Working modulo δ, the terms in $\gamma(a; b, c, d, e)$ go to 0, giving the remaining terms of $\phi(a; b, c, d, e)$ as the leading terms in the expression.

Potentially more interesting is the reduction to I_4 and $I_{2,2}$ in light of the folklore conjecture that indices 1 can always be eliminated from MPL's. For that, we can make use of the following identity

$$
I_{3,1}(x, y) \overset{ш}{=} \frac{1}{2}(I_{2,2}(y, x) - I_{2,2}(x, y)) \,,
$$

to obtain

Corollary 5.2.4 (Dan with $I_{2,2}$)**.** *As shorthand, write $abcd \coloneqq \mathrm{cr}(a, b, c, d)$, and $abc \coloneqq \mathrm{cr}(a, b, c, \infty)$. Also write $[x, y]_{2,2} = [0 \mid x, 0, y, 0 \mid 1]$ and $[x] \coloneqq [x]_4 = [0 \mid x, 0, 0, 0, \mid 1]$. Then modulo products*

$$
[a \mid b, c, d, e \mid f] = \phi(a; b, c, d, e) - \phi(f; b, c, d, e) \,,
$$

where $\phi(a; b, c, d, e)$ *is exactly as given in Equation 5.2.2, and we understand that the shorthand* $[x, y]$ *is now as follows*

$$[x, y] = \frac{1}{2}([y, x]_{2,2} - [x, y]_{2,2}) .$$

5.2.2 Relation to Dan's previous reduction, and $I_{3,1}$ functional equations

Recall that in Théorème 3 of [Dan08], Dan gives a different reduction for $I_{1,1,1,1}$ to $I_{3,1}$ and I_4 terms. This version is specific to the weight 4 case $I_{1,1,1,1}$, and produces a more symmetrical and structured identity. Nevertheless, there is a typo in the expression Dan gives, but fortunately one can take advantage of the extra structure to easily correct the result. The correction below was provided by Gangl.

Theorem 5.2.5 (Théorème 3 in [Dan08], corrected by Gangl)**.** *As shorthand, write* $abcd \coloneqq \operatorname{cr}(a, b, c, d)$, *and* $abc \coloneqq \operatorname{cr}(a, b, c, \infty)$. *Moreover, write* $[x, y] \coloneqq [x, y]_{3,1} = [0 \mid x, 0, 0, y \mid 1]$ *and* $[x] \coloneqq [x]_4 = [0 \mid x, 0, 0, 0, \mid 1]$. *Then modulo products*

$$[a \mid b, c, d, e \mid f] = f(a; b, c, d, e) - f(f; b, c, d, e) ,$$

where

$$\begin{aligned} 20f(a; b, c, d, e) \coloneqq{} & g(a, b, c, d, e) + \\ & - g(\infty, b, c, d, e) - g(a, \infty, c, d, e) - g(a, b, \infty, d, e) + \\ & - g(a, b, c, \infty, e) - g(a, b, c, d, \infty) + \\ & + 10h(a, b, c, d, e) . \end{aligned}$$

And g *and* h *are defined by*

$$\begin{aligned} g(a, b, c, d, e) &\coloneqq \operatorname{Cyc}_{\{\, a,b,c,d,e \,\}} \left([abcd, abce]_{3,1} - [edcb, edca]_{3,1} - 3[abdc, abde]_{3,1} + 3[edbc, edba]_{3,1}\right) \\ h(a, b, c, d, e) &\coloneqq \operatorname{Cyc}_{\{\, a,b,c,d,e \,\}} \left([cab]_4 + [bda]_4 + [adb]_4 + [bad]_4\right) . \end{aligned}$$

Remark 5.2.6. The mistakes in Dan's expression occur in the first summand of g, where he write $[abcd, bcde]_{3,1}$ rather than $[abcd, abce]_{3,1}$. This is easily corrected upon noticing that for the remaining summands, the first 3 cross-ratio slots agree in each pair – that is, each is a 'coupled cross-ratio'. There is also a mistake in (his equivalent of) h, where the sign of the third term $[adb]_4$ is flipped. Moreover there appears to be a global sign error, so -20 in the definition of f is replaced with 20 above.

Once Dan has these two reductions, he wonders how the combinations ϕ and f relate. By setting the two expressions equal, one obtains a functional equation reducing a certain combination of $I_{3,1}$'s to I_4's. Specifically there is the question of whether ϕ and f are exactly equal, and whether this functional equation, *a prior* of 4 variables, splits into two functional equations of 3 variables.

Using the symbol, we can answer this question as follows.

Claim 5.2.7. *The combinations $f(a;b,c,d,e)$ and $\phi(a;b,c,d,e)$ are not equal.*

Proof. If f and ϕ were equal, then their symbols modulo δ would also have to be equal. One can explicitly check using Mathematica [MA] that these symbols are different. Moreover, checking the symbol shows that $\phi(a;b,c,d,e)$ is *not* even cyclically symmetric, so there is no hope that f and ϕ agree. □

Nevertheless, by comparing the two expansions $\phi(a;b,c,d,e) - \phi(f;b,c,d,e) \overset{Ш}{=} [a \mid b,c,d,e \mid f] \overset{Ш}{=} f(a;b,c,d,e) - f(f;b,c,d,e)$, we obtain a functional equation relating a certain combination of $I_{3,1}$'s to I_4's, modulo products Ш. Unfortunately, the functional equation which results is not as interesting as one might hope. It reduces to a (complicated) combination of the following four basic functional equations, already given by Gangl in [Gan16]. (It is the sum of approximately 630 instances of these basic functional equations. The leftover I_4 terms cancel pairwise using $I_4(x) = -I_4(\frac{1}{x})$.)

Identity 5.2.8 (Gangl)**.** *Using the notation of Chapter 4, the following identities hold modulo Ш.*

$$\begin{aligned} &I_{3,1}((ab)cde) - I_{3,1}((ba)cde) + \\ &\quad - I_4(abcd) + I_4(abce) + 3I_4(abde) \overset{Ш}{=} 0 \end{aligned} \qquad (I_{3,1}\ ab)$$

$$\begin{aligned} &I_{3,1}(a(bc)de) - I_{3,1}(a(cb)de) + \\ &\quad + I_4(cbad) - I_4(cbae) + 2I_4(abde) + 2I_4(cade) + I_4(cbde) \overset{Ш}{=} 0 \end{aligned} \qquad (I_{3,1}\ bc)$$

$$I_{3,1}(abc(de)) + I_{3,1}(abc(ed)) \overset{Ш}{=} 0 \qquad (I_{3,1}\ de)$$

$$\begin{aligned} &I_{3,1}((abcd)e) + I_{3,1}((bcda)e) + I_{3,1}((cdab)e) + I_{3,1}((dabc)e) + \\ &\quad + I_4(acbe) + I_4(bdce) + I_4(cade) + I_4(dbae) + \\ &\quad + 2I_4(abde) + 2I_4(bcae) + 2I_4(cdbe) + 2I_4(dace) \overset{Ш}{=} 0 \end{aligned} \qquad (I_{3,1}\ \text{cyc})$$

In fact, this was to be expected. Gangl has found that these functional equations provide a basis for the space of all relations between $I_{3,1}(abcde)$ terms. Moreover, we know from Remark 5.2.3 that every term of the weight 4 reduction can be written in this form.

5.3 Reduction of $I_{1,1,1,1,1}$

We shall now apply Dan's reduction procedure to the quintuple-log $I_{1,1,1,1,1}(v,w,x,y,z)$ to obtain expressions for it in terms of lower depth multiple polylogarithms. Or rather we shall apply it to $H(a \mid b,c,d,e,f \mid g)$, like above. Firstly we will examine the 'raw' output of the reduction procedure which reduces $I_{1,1,1,1,1}$ to the 11 depth ≤ 3 integral $I_5, I_{4,1}, I_{3,2}, I_{3,1,1}, I_{2,2,1}, \ldots$. Then using some identities from Chapter 4, we will be able to reduce this expression to explicit $I_5, I_{3,2}, I_{3,1,1}$ terms only, modulo Ш.

In order to explicitly confirm the folklore conjecture that indices 1 can always be eliminated from MPL's, we need to reduce $I_{3,1,1}$ to $I_{3,2}$ terms and I_5 terms. Like the reduction of $I_{3,2}$ to $I_{4,1}$ modulo δ given in Identity 4.2.17, we can give a brute force reduction of $I_{3,1,1}$ in terms of $I_{3,2}$, modulo δ. Currently I am unable to find the missing Li_5 terms to give an reduction of $I_{3,1,1}$ to $I_{3,2}$ and I_5, modulo $\sqcup$. Nevertheless, this allows us to reduce $I_{1,1,1,1,1}$ to only $I_{3,2}$ terms, modulo δ, and reduces the problem of a full reduction to dealing only with the case $I_{3,1,1}$ in terms of $I_{3,2}$ and I_5. Moreover, an expression for $I_{3,2}$ in terms of $I_{4,1}$ and very complicated Li_5 terms does exist, as given in Section B.1. We therefore have cause for optimism in trying to find a similar expression for $I_{3,1,1}$ in terms of $I_{3,2}$ terms and Li_5 terms.

5.3.1 'Raw' output of $I_{1,1,1,1,1}$ reduction

When attempting to reduce $I_{1,1,1,1,1}$ with Dan's reduction method, there are two choices. We can either use the structured approach from Section 5.1.7.1 which works for all n. Or we can use the structured approach from Section 5.1.7.2 which works only for n odd. The n odd approach has the advantage of producing significantly shorter reductions. We will compare the two initial results to see how much better the n odd approach works.

All n approach: Apply the all n approach to $[a \mid b, c, d, e, f \mid g]$. The result can be written as $\phi'(a; b, c, d, e, f) - \phi'(g; b, c, d, e, f)$, where ϕ' consists of this terms which contain the variable a. We obtain the following distribution of terms in ϕ'.

Integral	Number of such terms in ϕ'
I_5	37
$I_{1,4}$	29
$I_{2,3}$	39
$I_{3,2}$	41
$I_{4,1}$	34
$I_{1,1,3}$	14
$I_{1,2,2}$	22
$I_{1,3,1}$	21
$I_{2,1,2}$	22
$I_{2,2,1}$	26
$I_{3,1,1}$	22
Total number	307

Odd n approach: Apply the odd n approach to $[a \mid b, c, d, e, f \mid g]$. The result can be written as $\psi(a; b, c, d, e, f) - \psi(g; b, c, d, e, f)$, where ψ consists of those terms which contain the variable a. We obtain the following distribution of terms in ψ.

Integral	Number of such terms in ψ
I_5	20
$I_{1,4}$	11
$I_{2,3}$	17
$I_{3,2}$	17
$I_{4,1}$	11
$I_{1,1,3}$	6
$I_{1,2,2}$	5
$I_{1,3,1}$	6
$I_{2,1,2}$	7
$I_{2,2,1}$	7
$I_{3,1,1}$	6
Total number	113

Already one can see that the n odd approach is significantly better as it involves only about one-third the number of terms, compared to the all n approach. This reduction of $I_{1,1,1,1,1}$ to depth ≤ 3 integrals is (just) short enough to give explicitly.

Identity 5.3.1. *As shorthand recall the 'coupled cross-ratio' notation from Section 4.1.2, which has $I_{n_1,\ldots,n_k}(abcd_1 \ldots d_k) \coloneqq I_{n_1,\ldots,n_k}(\operatorname{cr}(a,b,c,d_1),\ldots,\operatorname{cr}(a,b,c,d_k))$. Then modulo products, Dan's reduction procedure the following reduction*

$$[a \mid b,c,d,e,f \mid g] = \psi(a;b,c,d,e,f) - \psi(g;b,c,d,e,f)\,,$$

where

$$\begin{aligned}
&\psi(a;b,c,d,e,f) \coloneqq \\
&I_5(-[bdac] + 4[bdae] - [bdaf] + 4[bda\infty] - [bfac] + 4[bfad] - 6[bfae] + 4[bfa\infty] + \\
&\qquad + 6[d\infty ab] + [d\infty ac] - 4[d\infty ae] + [d\infty af] + [f\infty ab] + [f\infty ac] - 4[f\infty ad] + \\
&\qquad + 6[f\infty ae] + 2[\infty bac] + 2[\infty bad] + 2[\infty bae] + 2[\infty baf]) + \\
&+ I_{1,4}([bdac\infty] - [bdaef] + [bfacd] - 3[bfade] + 3[bfae\infty] - 3[d\infty abe] + \\
&\qquad + [d\infty aef] - [f\infty acd] + 3[f\infty ade] - [\infty bacd] + [\infty baef]) + \\
&+ I_{2,3}(-[bdaef] - 2[bda\infty e] + [bface] - [bfade] - 2[bfad\infty] + 2[bfae\infty] + \\
&\qquad - 2[d\infty abe] - [d\infty abf] - [d\infty acb] + [d\infty aef] - [f\infty ace] + [f\infty ade] + \\
&\qquad - [f\infty aeb] - [\infty bacd] - [\infty bace] - [\infty bade] - [\infty badf]) + \\
&+ I_{3,2}([bdace] - [bdaef] - 2[bda\infty e] - [bda\infty f] + [bfac\infty] - 2[bfad\infty] + \\
&\qquad + [bfae\infty] - [d\infty abe] - 2[d\infty abf] - [d\infty ace] + [d\infty aef] + [f\infty adb] + \\
&\qquad - 2[f\infty aeb] - [\infty bace] - [\infty bade] - [\infty badf] - [\infty baef]) + \\
&+ I_{4,1}([bdacf] - [bdaef] - 3[bda\infty f] - 3[d\infty abf] - [d\infty acf] + [d\infty aef] +
\end{aligned}$$

$$
\begin{aligned}
&- [f\infty acb] + 3[f\infty adb] - 3[f\infty aeb] - 2[\infty bacf] - 2[\infty baef]) + \\
&+ I_{1,1,3}(-[bfacde] + 2[bfade\infty] + [d\infty abef] + [f\infty acde] + [\infty bacde] + [\infty badef]) + \\
&+ I_{1,2,2}(-[bdac\infty e] - [bfacd\infty] + [bfade\infty] + [d\infty abef] - [f\infty adeb]) + \\
&+ I_{1,3,1}(-[bdac\infty f] + [d\infty abef] + [f\infty acdb] - 2[f\infty adeb] + [\infty bacdf] - [\infty badef]) + \\
&+ I_{2,1,2}([bda\infty ef] - [bface\infty] + [bfade\infty] + [d\infty abef] + [d\infty acbe] + [\infty bacde] + [\infty badef]) + \\
&+ I_{2,2,1}([bda\infty ef] + [d\infty abef] + [d\infty acbf] + [f\infty aceb] - [f\infty adeb] + [\infty bacdf] + [\infty bacef]) + \\
&+ I_{3,1,1}(-[bdacef] + 2[bda\infty ef] + [d\infty abef] + [d\infty acef] + [\infty bacef] + [\infty badef])\,.
\end{aligned}
$$

5.3.2 Reduction of $I_{1,1,1,1,1}$ to $I_{3,1,1}$, $I_{3,2}$ and I_5 modulo products

From Chapter 4, we have a number of identities which relate depth 2 and depth 3 iterated integrals. In particular, Proposition 4.2.22 allows us to write $I_{1,4}$ as $I_{4,1}$, and write $I_{2,3}$ as $I_{3,2}$. Then Equation 4.2.7b in Identity 4.2.16 allows us to write $I_{4,1}$ as a sum of $I_{3,2}$ terms.

Moreover, Theorem 4.3.18 tells us that all depth 3 interated integrals are somehow 'equivalent' modulo $I_{3,2}$. In particular, every such integral can be written as $I_{3,1,1}$. We can use Identity 4.3.16, and Identity 4.3.20 to explicitly reduce $I_{1,3,1}$ and $I_{2,2,1}$ to $I_{3,1,1}$, modulo products. We can also use Identity 4.3.19, but we first need to add in the missing Li_5, or rather I_5, terms. We have

Identity 5.3.2. *We can find I_5 terms for Identity 4.3.19, to give the following identity relating $I_{1,1,3}$ to $I_{3,1,1}$, modulo products, with explicit $I_{3,2}$ and I_5 terms.*

$$
\begin{aligned}
I_{3,1,1}(abcdef) - I_{1,1,3}(abdcfe) \overset{\sqcup\!\sqcup}{=} \frac{1}{3} I_{3,2}(&-[abdfe] - [abfce] - [abfde] - [abfed] + \\
&- [baefd] + [bafec] + [bafed]) + \\
&+ \frac{1}{3} I_5(-16[abed] + 4[abfd] - 7[abfe] - 6[abce] + 4[abcf])
\end{aligned}
$$

To complete the reduction to $I_{3,1,1}$, $I_{3,2}$ and I_5, we need to give a reduction for $I_{2,1,2}$ and $I_{1,2,2}$ to $I_{3,1,1}$, $I_{3,2}$ and I_5. Theorem 4.3.18 shows that this can certainly be done, modulo $I_{3,2}$, then we could attempt to find the missing I_5 terms. Alternatively, one can more directly find the the following identities.

Identity 5.3.3. *The following identity expresses $I_{2,1,2}$ in terms of $I_{3,1,1}$ terms, $I_{3,2}$ terms, and I_5 terms, modulo products.*

$$
\begin{aligned}
&I_{2,1,2}(abcdef) \overset{\sqcup\!\sqcup}{=} \\
&I_{3,1,1}([abcdfe] + [abcfde] + [abcfed] + [abdcef] + [abdecf] + [abedcf]) + \\
&+ I_{3,2}([abcdf] + 2[abcef] - [abcfd] - [abcfe] + [abdcf] + [abdef] + \\
&+ 2[abecf] + [abedf] - [abefc]) + I_5(12[abcf] + 6[abdf] + 12[abef])
\end{aligned}
$$

Identity 5.3.4. *The following identity expresses $I_{1,2,2}$ in terms of $I_{3,1,1}$ terms, $I_{3,2}$ terms, and I_5*

terms, modulo products.

$$\begin{aligned}
&I_{1,2,2}(abcdef) \overset{\sqcup\!\sqcup}{=} \\
&I_{3,1,1}(-[abcfed] - [abdcef] - [abdcfe] - [abdecf]) + \\
&+ I_{3,2}(-2[abcef] + [abcfe] - 2[abecf] - [abefd] - [abfed]) + \\
&+ I_5(-12[abcf] - 6[abde] - 6[abdf] - 6[abef])
\end{aligned}$$

Applying the above identities to ψ from Identity 5.3.1 produces $\psi'(a; b, c, d, e, f)$ with the following distribution of terms. The explicit expression for ψ' is given in the appendix, in Section B.3.

Integral	Number of such terms in ψ'
I_5	50
$I_{3,2}$	125
$I_{3,1,1}$	69
Total number	244

5.3.3 Reduction of $I_{1,1,1,1,1}$ to $I_{3,2}$ modulo δ

Ideally, the final step would be to give some way to write $I_{3,1,1}$ in terms of $I_{3,2}$ and I_5 modulo products. That way we can completely reduce $I_{1,1,1,1,1}$ to $I_{3,2}$ and I_5, and explicitly confirm that the index 1 can always be eliminated. Unfortunately the I_5 terms in this step have remained elusive. Nevertheless, we have the following identity which expresses $I_{3,1,1}$ in terms of $I_{3,2}$ modulo δ.

Identity 5.3.5. *The following identity expresses $I_{3,1,1}(abcdef) \leftrightarrow I_{3,1,1}(x, y, z)$ in terms of $I_{3,2}$ terms, modulo δ.*

$$\begin{aligned}
&3I_{3,1,1}(abcdef) \overset{\delta}{=} \\
&+ I_{3,2}([abcde] + [abcdf] + [abced] + [abcfd] - [acbdf] - [acbfd] - [adbef] + \\
&\quad - [adbfe] + [bafce] + [bafec] - [bface] - [bfaec]) + \\
&+ I_{3,2}([abce, acbd] + [abce, adbc] + [abcf, adcb] - [abdf, aebf] - [abef, adeb] + \\
&\quad - [abef, aedb] + [acbd, abce] + [adbc, abce] - [adbc, abfc] + [adbe, abfe] + \\
&\quad - [adbf, aebd] + [aebd, abfe] - [aebd, adbf] - [aebf, abdf]) + \\
&+ I_{3,2}([abcd, abfe] - [abef, abdc] - [abef, adbc] + [acbd, aecf] - [acbd, bcef] + \\
&\quad - [acbd, becf] - [acdf, adbe] - [acdf, aebd] + [acdf, aebf] - [acef, adbc] + \\
&\quad + [acef, adbe] + [acef, aebd] - [adbc, abef] - [adbc, acef] - [adbe, acdf] + \\
&\quad + [adbe, acef] - [aebd, acdf] + [aebd, acef] + [aebf, acdf] + [aecf, acbd] + \\
&\quad + [afbe, bcdf] + [bcdf, afbe] - [bcef, acbd] - [becf, acbd])
\end{aligned}$$

Remark 5.3.6. In this identity, the $I_{3,2}$ terms are grouped (roughly) according to their complexity. Initially we have 12 terms of the form $I_{3,2}(abcde)$, which constitute 'coupled cross-ratios'. One should think of these as the simplest kind of term. Then we have 14 terms of the form $I_{3,2}(abce, acbd)$; these do not exactly fit the form of a 'coupled cross-ratio', but they do involve only 5 of the 6 variables $abcdef$. This makes them of intermediate complexity. Lastly, we have 24 terms of the form $I_{3,2}(abcd, abef)$, which contain all 6 of the variables in each term. These are the most complex type of term.

Remark 5.3.7. The above identity expresses $I_{3,1,1}$ in terms of 50 $I_{3,2}$ terms. Slightly shorter expressions are possible, but they involve coefficients ± 1 and $\pm\frac{1}{2}$, rather than just ± 1, as above. In terms of generating (or rather not generating) a 'useful' final expression for $I_{1,1,1,1,1}$ in terms of $I_{3,2}$, choosing the longer expression over the shorter one makes little difference.

The expression for $I_{3,1,1}$ in terms of $I_{3,2}$ holds modulo δ. One would hope to be able to find Li_5 terms which make the identity hold modulo products only. So far this has been unsuccessful. But given the existence of the Li_5 terms in Identity B.1.1, which make the brute-force expression for $I_{3,2}$ in terms of $I_{4,1}$'s from Identity 4.2.17 hold, modulo products, one is optimistic that Li_5 terms to make Identity 5.3.5 hold, modulo products, *do* exist.

If we apply Identity 5.3.5 to the ψ' found in Section 5.3.2 (and given explicitly in Theorem B.3.1), we obtain the following.

Theorem 5.3.8. *Modulo δ, we can write*

$$[a \mid b, c, d, e, f \mid g] = \psi''(a; b, c, d, e, f) - \psi''(g; b, c, d, e, f)\,,$$

where ψ'' is an explicit *combination of the following type of $I_{3,2}$ terms:*

- *'Coupled cross-ratio terms' $I_{3,2}(abcde)$,*
- *5-variable cross-ratio terms $I_{3,2}(abcd, abde)$, and*
- *6-variable cross-ratio terms $I_{3,2}(abcd, abef)$.*

Remark 5.3.9. In each case of Theorem 5.3.8 above, (viewing $[abcde] = [abcd, abce]$), the number of cross-ratios which have a variable set to infinity is either 0, 1, or 2. Moreover, the expression obtained for ψ'' by applying Identity 5.3.5 to Theorem B.3.1, has the following distribution of terms.

Integral	Number of ∞ cross-ratios	Number of such terms in ψ''
Coupled cross-ratio $I_{3,2}$	0	68
Coupled cross-ratio $I_{3,2}$	1	88
Coupled cross-ratio $I_{3,2}$	2	276
5-variable cross-ratio $I_{3,2}$	0	78
5-variable cross-ratio $I_{3,2}$	1	155
5-variable cross-ratio $I_{3,2}$	2	578
6-variable cross-ratio $I_{3,2}$	0	48
6-variable cross-ratio $I_{3,2}$	1	686
6-variable cross-ratio $I_{3,2}$	2	480
Total number		2457

Chapter 6

Arbitrary weight $I_{a,b}(x,y) \pm I_{a,b}(\frac{1}{x},\frac{1}{y})$ inversion identity

This chapter will focus on proving a generalisation of an identity found in [Gan16] in the weight 4 case, and in Chapter 4 in the the weight 5 case. The identity (Theorem 6.1.2) concerns the products and Li_n terms which complete $I_{a,b}(x,y) \pm I_{a,b}(\frac{1}{x},\frac{1}{y}) \overset{\delta}{=} 0$ to an identity holding on the level of the symbol.

The proof of the general identity will involve a long and tedious calculation using the symbol of $I_{a,b}(x,y)$. It will be convenient to use the symbol for $I_{a,b}(x,y)$ as computed by Rhodes [Rho12], but first we want to make some simplifications (Section 6.2.2). The proof then proceeds by computing the symbol of the left hand side (Section 6.2.3), and of the right hand side (Section 6.2.5). Comparing both sides (Section 6.2.6) after 'gathering' by the first tensor factor in each term completes the proof.

Finally we attempt to upgrade the subfamily $I_{n,1}(x,y) \pm I_{n,1}(\frac{1}{x},\frac{1}{y})$ to a candidate numerically testable family of identities holding at arbitrary weight, mimicking the approached used in the weight 4 case by Duhr (related by Gangl [Gan16]). To do this we need to compute refinements incorporating constant $\times$ lower weight terms which are invisible on the level of the symbol, but show up in the coproduct. We compute slices $\Delta_{k,1,\ldots,1}$ of the coproduct to explicitly find the weight 5 identity (Section 6.3.2) and the weight 6 identity (Section 6.3.3). Enough of a pattern is apparent across the weight 4, 5 and 6 cases to suggest an arbitrary weight numerically testable identity (Section 6.3.4), which passes various numerical tests.

Addendum: we also point recent work by Panzer ('Parity theorem for multiple polylogarithms' [Pan15]) which has subsumed the identities in this chapter, giving a numerically verifiable inversion identity for any multiple polylogarithm $\mathrm{Li}_{n_1,\ldots,n_d}$ of any depth, and of any indices.

6.1 Buildup to the identity

From various results when investigating symmetries and relations between weight 5 MPL's, it seems to be the case that for any depth 2 iterated integral $I_{a,b}(x,y)$, we always have the following symmetry.

$$I_{a,b}(x,y) - (-1)^{a+b} I_{a,b}(\tfrac{1}{x},\tfrac{1}{y}) \overset{\delta}{=} 0\,.$$

See for example Equation 4.2.1b′ for the case $I_{4,1}$, and Equation 4.2.4′ for the case $I_{3,2}$.

Moreover, the leading order Li_n terms can be found in enough explicit cases to suggest the following general expression.

$$\begin{aligned}&I_{a,b}(x,y) - (-1)^{a+b} I_{a,b}(\tfrac{1}{x},\tfrac{1}{y}) \\ &\overset{\text{ш}}{=} (-1)^{a+b}\,\mathrm{Li}_{a+b}(x) + (-1)^b \tbinom{a+b-1}{a}\,\mathrm{Li}_{a+b}(y) - (-1)^a \tbinom{a+b-1}{b}\,\mathrm{Li}_{a+b}(\tfrac{x}{y})\,.\end{aligned}$$

For this, see Identity 4.2.7 and Identity 4.2.13

The next natural step is to find the missing product terms, so that we may give a symbol-level identity on the nose. It is possible to do this in each of these cases, and enough of a pattern is present to suggest a general identity. One such case is available in Identity 4.2.8.

Before stating the symbol-level identity, it is helpful to introduce some notation which will (slightly) simplify the calculation of the symbol later.

Definition 6.1.1. Let $\alpha \in \mathbb{Z}_{\geq 0}$. Then write

$$\widetilde{\log}^{\alpha}(x) \coloneqq \tfrac{1}{\alpha!}\log^{\alpha}(x)\,.$$

In the case where $\alpha = 0$, this is interpreted as

$$\widetilde{\log}^{0}(x) = \tfrac{1}{0!}\log^{0}(x) = 1\,.$$

Theorem 6.1.2. *For any $a, b \in \mathbb{Z}_{>0}$, the following identity holds exactly on the level of the symbol.*

$$I_{a,b}(x,y) - (-1)^{a+b} I_{a,b}(\tfrac{1}{x},\tfrac{1}{y}) \quad \overset{\mathcal{S}}{=} \tag{6.1.1a}$$

$$(-1)^b \sum_{i=0}^{a} \tbinom{b-1+i}{i} (\widetilde{\log}(\tfrac{1}{x}))^{a-i}\,\widetilde{\log}(y)^{b+i} + \tag{6.1.1b}$$

$$+ (-1)^b \sum_{i=0}^{a} \tbinom{b-1+i}{i} (\widetilde{\log}(\tfrac{1}{x}))^{a-i}\,\mathrm{Li}_{b+i}(y) + \tag{6.1.1c}$$

$$- (-1)^a \sum_{i=0}^{b} \tbinom{a-1+i}{i} (\widetilde{\log}(\tfrac{1}{x}))^{b-i}\,\mathrm{Li}_{a+i}(\tfrac{x}{y}) + \tag{6.1.1d}$$

$$+ (-1)^{a+b}\,\mathrm{Li}_a(\tfrac{x}{y})\,\widetilde{\log}^{b}(y) + (-1)^{a+b}\,\mathrm{Li}_{a+b}(x)\,. \tag{6.1.1e}$$

In particular, we have the leading terms

$$I_{a,b}(x,y) - (-1)^{a,b} I_{a,b}(\tfrac{1}{x},\tfrac{1}{y}) \overset{\text{ш}}{=}$$

$$(-1)^b \binom{a+b-1}{a} \operatorname{Li}_{a+b}(y) - (-1)^a \binom{a+b-1}{b} \operatorname{Li}_{a+b}(\tfrac{x}{y}) + (-1)^{a+b} \operatorname{Li}_{a+b}(x) \,.$$

The following section is devoted to proving this identity on the level of the symbol. The reader uninterested in working through the details may skip to Section 6.3, where the identity for $I_{n,1}$ will be lifted up to a numerically testable identity.

6.2 Proof of the identity

The proof of the identity will be a direct calculation of the symbol of both sides. In order to calculate the LHS, I need to use the symbol of $I_{a,b}(x,y)$ as computed by Rhodes [Rho12]. In fact, I want to use a 'simplified' version of it, and in order to make the simplification we need some auxiliary results.

Warning 6.2.1. In the calculations that follow, we are working with multiplicative tensors from the symbol. So we cannot write 1 for the empty word (tensor of length 0) because $1 \in \mathbb{Q}(x)^{\otimes 1}$ is a perfectly good tensor factor. Moreover, in the symbol terms of the form $\cdots \otimes 1 \otimes \cdots$ vanish. Therefore we shall use $\emptyset$ to refer to the empty word.

6.2.1 Some lemmas

The auxiliary results needed are the following.

Lemma 6.2.2. *Let Γ be a tensor of some length, and let α, β some single tensor factors. We have*

$$\begin{aligned} \alpha^{\otimes t} ⧢ (\beta \otimes \Gamma) &= \sum_{j=0}^{t} \alpha^{\otimes j} \otimes \beta \otimes (\alpha^{\otimes t-j} ⧢ \Gamma) \\ &= \sum_{i+j=t} \alpha^{\otimes i} \otimes \beta \otimes (\alpha^{\otimes j} ⧢ \Gamma) \,. \end{aligned}$$

Proof. This follows by induction using the recursive definition of ⧢. That definition says

$$(\alpha \otimes \Gamma) ⧢ (\beta \otimes \Delta) = \alpha \otimes (\Gamma ⧢ (\beta \otimes \Delta)) + \beta \otimes ((\alpha \otimes \Gamma) ⧢ \Delta) \,,$$

where Γ, Δ are tensors of some length, and α, β are length 1 tensor factors.

The lemma is true for $t = 0$, in which case both sides reduce to $\beta \otimes \Gamma$, since $\emptyset ⧢ \Delta = \Delta$. Now assume we have the statement for t. Then for $t+1$ we find

$$\begin{aligned} \alpha^{\otimes t+1} ⧢ (\beta \otimes \Gamma) &= \alpha \otimes (\alpha^{\otimes t} ⧢ (\beta \otimes \Gamma)) + \beta \otimes (\alpha^{\otimes t+1} ⧢ \Gamma) \\ &= \alpha \otimes \sum_{j=0}^{t} \alpha^{\otimes j} \otimes \beta \otimes (\alpha^{\otimes t-j} ⧢ \Gamma) + \beta \otimes (\alpha^{\otimes t+1} ⧢ \Gamma) \\ &= \sum_{j=0}^{t} \alpha^{\otimes j+1} \otimes \beta \otimes (\alpha^{\otimes t-j} ⧢ \Gamma) + \beta \otimes (\alpha^{\otimes t+1} ⧢ \Gamma) \\ &= \sum_{j=1}^{t+1} \alpha^{\otimes j} \otimes \beta \otimes (\alpha^{\otimes t+1-j} ⧢ \Gamma) + \underbrace{\beta \otimes (\alpha^{\otimes t+1} ⧢ \Gamma)}_{j = 0 \text{ term of the sum}} \end{aligned}$$

$$= \sum_{j=0}^{t+1} \alpha^{\otimes j} \otimes \beta \otimes (\alpha^{\otimes t-j} \sqcup\!\sqcup \Gamma)\,.$$

So by induction the result holds. □

Lemma 6.2.3. *We have*

$$\sum_{i+j=N} \alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes j} = (\alpha\beta)^{\otimes N}\,.$$

Proof. This certainly holds for $N = 0$ since both sides reduce to the empty word $\emptyset$.

Now consider the case $N + 1$. We have

$$\begin{aligned}
(\alpha\beta)^{\otimes N+1} &= (\alpha\beta) \otimes (\alpha\beta)^{\otimes N} \\
&= ([\alpha] + [\beta]) \otimes \sum_{i=0}^{N} \alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N-i} \\
&= \sum_{i=0}^{N} \alpha \otimes (\alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N-i}) + \sum_{i=0}^{N} \beta \otimes (\alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N-i})\,.
\end{aligned}$$

Reindex the first sum to obtain

$$\begin{aligned}
&= \sum_{i=1}^{N+1} \alpha \otimes (\alpha^{\otimes i-1} \sqcup\!\sqcup \beta^{\otimes N+1-i}) + \sum_{i=0}^{N} \beta \otimes (\alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N-i}) \\
&= \alpha \otimes (\alpha^{\otimes N} \sqcup\!\sqcup \emptyset) + \sum_{i=1}^{N} \alpha \otimes (\alpha^{\otimes i-1} \sqcup\!\sqcup \beta^{\otimes N+1-i}) \\
&\quad + \sum_{i=1}^{N} \beta \otimes (\alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N-i}) + \beta \otimes (\emptyset \sqcup\!\sqcup \beta^{N})
\end{aligned}$$

By the recursive definition of $\sqcup\!\sqcup$ we have

$$\alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N+1-i} = \alpha \otimes (\alpha^{\otimes i-1} \sqcup\!\sqcup \beta^{\otimes N+1-i}) + \beta \otimes (\alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N-i})\,.$$

This means we can combine the two summations above as follows, to get

$$\begin{aligned}
&\alpha \otimes (\alpha^{\otimes N} \sqcup\!\sqcup \emptyset) + \sum_{i=1}^{N} \alpha \otimes (\alpha^{\otimes i-1} \sqcup\!\sqcup \beta^{\otimes N+1-i}) \\
&\qquad + \sum_{i=1}^{N} \beta \otimes (\alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N-i}) + \beta \otimes (\emptyset \sqcup\!\sqcup \beta^{\otimes N}) \\
&= \alpha^{\otimes N+1} \sqcup\!\sqcup \emptyset + \sum_{i=1}^{N} \alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N+1-i} + \emptyset \sqcup\!\sqcup \beta^{\otimes N+1} \\
&= \sum_{i=0}^{N+1} \alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes N+1-i} \\
&= \sum_{i+j=N+1} \alpha^{\otimes i} \sqcup\!\sqcup \beta^{\otimes j}\,.
\end{aligned}$$

We obtain the result for $N + 1$. So by induction the lemma is proved. □

6.2.2 Symbol of $I_{a,b}(x,y)$

We can use the above results to find a convenient expression for the symbol of $I_{a,b}(x,y)$. We'll use this to assemble the symbol of the LHS.

From Theorem 4.9 in Rhodes [Rho12], we have that the symbol of the iterated integral $I_{a,b}(x,y)$ is given by the following. Here we use the convention that $\sqcup\!\sqcup$ has higher precedence than $\otimes$.

$$\mathcal{S}(I_{a,b}(x,y)) = \sum_{t_1+t_2=a-1} (-1)^{t_1+b-1} \left[(1-\tfrac{1}{y}) \otimes y^{\otimes b-1} \sqcup\!\sqcup \left((1-\tfrac{y}{x}) \otimes x^{\otimes t_1} \sqcup\!\sqcup y^{\otimes t_2}\right)\right] \tag{6.2.1a}$$

$$+ \sum_{\substack{t_1+t_2=a-1\\t_3+t_4=b-1}} (-1)^{t_1+b} \binom{t_2+t_4}{t_2} \left[(1-\tfrac{1}{x}) \otimes x^{\otimes t_3} \otimes (1-\tfrac{x}{y}) \otimes y^{\otimes t_2+t_4} \sqcup\!\sqcup x^{\otimes t_1}\right] \tag{6.2.1b}$$

$$+ \sum_{t_1+t_2=a-1} (-1)^{t_1+b+1} \binom{t_2+b-1}{t_2} \left[(1-\tfrac{1}{x}) \otimes x^{\otimes t_1} \sqcup\!\sqcup \left((1-\tfrac{1}{y}) \otimes y^{\otimes t_2+b-1}\right)\right] \tag{6.2.1c}$$

Let's simplify this and put it into a more useful form.

First term of $\mathcal{S}(I_{a,b}(x,y))$: Let's look at the first term in the symbol of $I_{a,b}(x,y)$, Equation 6.2.1a above. It is

$$\sum_{t_1+t_2=a-1} (-1)^{t_1+b-1} \left[(1-\tfrac{1}{y}) \otimes y^{\otimes b-1} \sqcup\!\sqcup \left((1-\tfrac{y}{x}) \otimes x^{\otimes t_1} \sqcup\!\sqcup y^{\otimes t_2}\right)\right] .$$

We can combine the $(-1)^{t_1}$ and $x^{\otimes t_1}$ to get $(\frac{1}{x})^{\otimes t_1}$. Similarly the $(-1)^{b-1}$ and $y^{\otimes b-1}$ to get $(\frac{1}{y})^{\otimes b-1}$. So the term becomes

$$\begin{aligned} &\sum_{t_1+t_2=a-1} (1-\tfrac{1}{y}) \otimes (\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup \left((1-\tfrac{y}{x}) \otimes (\tfrac{1}{x})^{\otimes t_1} \sqcup\!\sqcup y^{\otimes t_2}\right) \\ &= (1-\tfrac{1}{y}) \otimes (\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup \left((1-\tfrac{y}{x}) \otimes \sum_{t_1+t_2=a-1} (\tfrac{1}{x})^{\otimes t_1} \sqcup\!\sqcup y^{\otimes t_2}\right) . \end{aligned}$$

Then using Lemma 6.2.3 to evaluate the sum of shuffles gives

$$= (1-\tfrac{1}{y}) \otimes (\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup \left((1-\tfrac{y}{x}) \otimes (\tfrac{y}{x})^{\otimes a-1}\right) .$$

Finally using Lemma 6.2.2, we can write this as

$$= \sum_{i=0}^{b-1} (1-\tfrac{1}{y}) \otimes (\tfrac{1}{y})^{\otimes i} \otimes (1-\tfrac{y}{x}) \otimes \left((\tfrac{1}{y})^{\otimes b-1-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1}\right) .$$

Second term of $\mathcal{S}(I_{a,b}(x,y))$: The second term of the symbol of $I_{a,b}(x,y)$, Equation 6.2.1b, is

$$\sum_{\substack{t_1+t_2=a-1\\t_3+t_4=b-1}} (-1)^{t_1+b} \binom{t_2+t_4}{t_2} \left[(1-\tfrac{1}{x}) \otimes x^{\otimes t_3} \otimes (1-\tfrac{x}{y}) \otimes y^{\otimes t_2+t_4} \sqcup\!\sqcup x^{\otimes t_1}\right] .$$

Firstly, combine $(-1)^{t_1}$ and $x^{\otimes t_1}$ as before. Now use that

$$\alpha^{\otimes a} \sqcup\!\sqcup \alpha^{\otimes b} = \binom{a+b}{a} \alpha^{\otimes a+b} ,$$

to combine the binomial coefficient with $y^{\otimes t_2+t_4}$ and get

$$= \sum_{\substack{t_1+t_2=a-1\\t_3+t_4=b-1}} (-1)^b \left[(1-\tfrac{1}{x}) \otimes x^{\otimes t_3} \otimes (1-\tfrac{x}{y}) \otimes \left(y^{\otimes t_4} ⧢ y^{\otimes t_2} ⧢ (\tfrac{1}{x})^{\otimes t_1}\right)\right].$$

Since $t_3+t_4 = b-1$, we can combine $(-1)^{b-1}$ with $x^{\otimes t_3}$ and $y^{\otimes t_4}$ to get

$$= -\sum_{\substack{t_1+t_2=a-1\\t_3+t_4=b-1}} (1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes t_3} \otimes (1-\tfrac{x}{y}) \otimes \left((\tfrac{1}{y})^{\otimes t_4} ⧢ y^{\otimes t_2} ⧢ (\tfrac{1}{x})^{\otimes t_1}\right).$$

Since ⧢ is associative, we can bracket off $y^{\otimes t_2} ⧢ (\frac{1}{x})^{\otimes t_1}$ and evaluate the sum over $t_1+t_2 = a-1$ using Lemma 6.2.3. We get

$$\begin{aligned} &= -\sum_{t_3+t_4=b-1} (1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes t_3} \otimes (1-\tfrac{x}{y}) \otimes \left((\tfrac{1}{y})^{\otimes t_4} ⧢ (\tfrac{y}{x})^{\otimes a-1}\right) \\ &= -\sum_{i=0}^{b-1}(1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1-\tfrac{x}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-1-i} ⧢ (\tfrac{y}{x})^{\otimes a-1}\right) \end{aligned}$$

Third term of $\mathcal{S}(I_{a,b}(x,y))$: The third term of the symbol of $I_{a,b}(x,y)$, Equation 6.2.1c, is

$$\sum_{t_1+t_2=a-1} (-1)^{t_1+b+1}\binom{t_2+b-1}{t_2} \left[(1-\tfrac{1}{x}) \otimes x^{\otimes t_1} ⧢ \left((1-\tfrac{1}{y}) \otimes y^{\otimes t_2+b-1}\right)\right].$$

Combine the binomial coefficient with $y^{\otimes t_2+b-1}$, take $(-1)^{t_1}$ into $x^{\otimes t_1}$, and $(-1)^{b-1}$ into $y^{\otimes b-1}$ to get

$$= \sum_{t_1+t_2=a-1} (1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes t_1} ⧢ \left((1-\tfrac{1}{y}) \otimes \left(y^{\otimes t_2} ⧢ (\tfrac{1}{y})^{\otimes b-1}\right)\right)$$

Use Lemma 6.2.2 on the outer shuffle product, and we get

$$= \sum_{t_1=0}^{a-1}\sum_{i=0}^{t_1}(1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes j} \otimes (1-\tfrac{1}{y}) \otimes \left((\tfrac{1}{x})^{\otimes t_1-i} ⧢ y^{\otimes a-1-t_1} ⧢ (\tfrac{1}{y})^{\otimes b-1}\right).$$

Now interchange the order of summation, and reindex the sum over t_1 to start at $t_1 = 0$. This gives

$$\begin{aligned} &= \sum_{i=0}^{a-1}\sum_{t_1=i}^{a-1}(1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1-\tfrac{1}{y}) \otimes \left((\tfrac{1}{x})^{\otimes t_1-i} ⧢ y^{\otimes a-1-t_1} ⧢ (\tfrac{1}{y})^{\otimes b-1}\right) \\ &= \sum_{i=0}^{a-1}\sum_{t_1=0}^{a-1-i}(1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1-\tfrac{1}{y}) \otimes \left((\tfrac{1}{x})^{\otimes t_1} ⧢ y^{\otimes a-1-i-t_1} ⧢ (\tfrac{1}{y})^{\otimes b-1}\right). \end{aligned}$$

Finally, deal with the sum over t_1 using Lemma 6.2.3, and we get

$$\begin{aligned} &= \sum_{i=0}^{a-1}(1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1-\tfrac{1}{y}) \otimes \left((\tfrac{y}{x})^{\otimes a-1-i} ⧢ (\tfrac{1}{y})^{\otimes b-1}\right) \\ &= \sum_{i=0}^{a-1}(1-\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1-\tfrac{1}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a-1-i}\right) \end{aligned}$$

Conclusion: Combining these pieces shows that the symbol of $I_{a,b}(x,y)$ may be expressed as the following.

$$\begin{aligned}\mathcal{S}(I_{a,b}(x,y)) = &\sum_{i=0}^{b-1}(1-\tfrac{1}{y})\otimes(\tfrac{1}{y})^{\otimes i}\otimes(1-\tfrac{y}{x})\otimes\Big((\tfrac{1}{y})^{\otimes b-1-i}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1}\Big)\\ &-\sum_{i=0}^{b-1}(1-\tfrac{1}{x})\otimes(\tfrac{1}{x})^{\otimes i}\otimes(1-\tfrac{x}{y})\otimes\Big((\tfrac{1}{y})^{\otimes b-1-i}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1}\Big)\\ &+\sum_{i=0}^{a-1}(1-\tfrac{1}{x})\otimes(\tfrac{1}{x})^{\otimes i}\otimes(1-\tfrac{1}{y})\otimes\Big((\tfrac{1}{y})^{\otimes b-1}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1-i}\Big)\end{aligned}$$

6.2.3 Symbol of LHS

Now use the above expression for $\mathcal{S}(I_{a,b}(x,y))$ to compute $\mathcal{S}(-(-1)^{a+b}I_{a,b}(\frac{1}{x},\frac{1}{y}))$. When we write down the symbol of $-(-1)^{a+b}I_{a,b}(\frac{1}{x},\frac{1}{y})$, we can immediately re-invert the terms $(\frac{y}{x}),(\frac{1}{x}),(\frac{1}{y})$ using $(-1)^{a-1}$ and $(-1)^{b-1}$. This gives

$$\begin{aligned}\mathcal{S}(-(-1)^{a+b}I_{a,b}(\tfrac{1}{x},\tfrac{1}{y})) = &-\sum_{i=0}^{b-1}(1-y)\otimes(\tfrac{1}{y})^{\otimes i}\otimes(1-\tfrac{x}{y})\otimes\Big((\tfrac{1}{y})^{\otimes b-1-i}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1}\Big)+\\ &+\sum_{i=0}^{b-1}(1-x)\otimes(\tfrac{1}{x})^{\otimes i}\otimes(1-\tfrac{y}{x})\otimes\Big((\tfrac{1}{y})^{\otimes b-1-i}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1}\Big)+\\ &-\sum_{i=0}^{a-1}(1-x)\otimes(\tfrac{1}{x})^{\otimes i}\otimes(1-y)\otimes\Big((\tfrac{1}{y})^{\otimes b-1}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1-i}\Big)\,.\end{aligned}$$

The sum of these two expressions gives the symbol of the LHS

$$\begin{aligned}\mathcal{S}(\text{Equation 6.1.1 LHS}) = &\sum_{i=0}^{b-1}(1-\tfrac{1}{y})\otimes(\tfrac{1}{y})^{\otimes i}\otimes(1-\tfrac{y}{x})\otimes\Big((\tfrac{1}{y})^{\otimes b-1-i}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1}\Big)+ &\text{(6.2.2a)}\\ &-\sum_{i=0}^{b-1}(1-\tfrac{1}{x})\otimes(\tfrac{1}{x})^{\otimes i}\otimes(1-\tfrac{x}{y})\otimes\Big((\tfrac{1}{y})^{\otimes b-1-i}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1}\Big)+ &\text{(6.2.2b)}\\ &+\sum_{i=0}^{a-1}(1-\tfrac{1}{x})\otimes(\tfrac{1}{x})^{\otimes i}\otimes(1-\tfrac{1}{y})\otimes\Big((\tfrac{1}{y})^{\otimes b-1}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1-i}\Big)+ &\text{(6.2.2c)}\\ &-\sum_{i=0}^{b-1}(1-y)\otimes(\tfrac{1}{y})^{\otimes i}\otimes(1-\tfrac{x}{y})\otimes\Big((\tfrac{1}{y})^{\otimes b-1-i}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1}\Big)+ &\text{(6.2.2d)}\\ &+\sum_{i=0}^{b-1}(1-x)\otimes(\tfrac{1}{x})^{\otimes i}\otimes(1-\tfrac{y}{x})\otimes\Big((\tfrac{1}{y})^{\otimes b-1-i}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1}\Big)+ &\text{(6.2.2e)}\\ &-\sum_{i=0}^{a-1}(1-x)\otimes(\tfrac{1}{x})^{\otimes i}\otimes(1-y)\otimes\Big((\tfrac{1}{y})^{\otimes b-1}\sqcup\!\sqcup(\tfrac{y}{x})^{\otimes a-1-i}\Big)\,. &\text{(6.2.2f)}\end{aligned}$$

6.2.4 Towards the symbol of RHS

For ease of reference, I will reproduce here the RHS of the purported identity. It reads

$$(-1)^b\sum_{i=0}^{a}\binom{b-1+i}{i}(\widetilde{\log}(\tfrac{1}{x}))^{a-i}\,\widetilde{\log}(y)^{b+i}+ \tag{6.2.3a}$$

$$+ (-1)^b \sum_{i=0}^{a} \tbinom{b-1+i}{I} (\widetilde{\log}(\tfrac{1}{x}))^{a-i} \operatorname{Li}_{b+i}(y) + \tag{6.2.3b}$$

$$- (-1)^a \sum_{i=0}^{b} \tbinom{a-1+i}{(} \widetilde{\log}(\tfrac{1}{x}))^{b-i} \operatorname{Li}_{a+i}(\tfrac{x}{y}) + \tag{6.2.3c}$$

$$+ (-1)^{a+b} \operatorname{Li}_a(\tfrac{x}{y}) \widetilde{\log}^b(y) + \tag{6.2.3d}$$

$$+ (-1)^{a+b} \operatorname{Li}_{a+b}(x) \,. \tag{6.2.3e}$$

Let's write down the symbol of each term. Firstly, notice that

$$\mathcal{S}(\widetilde{\log}(x)^n) = \frac{1}{n!} x^{\sqcup\!\sqcup n} = \frac{1}{n!} n! x^{\otimes n} = x^{\otimes n} \,.$$

The notation $\widetilde{\log}(x)^n$ was introduced precisely for this reason.

When $n = 0$, we get the expected results: $x^{\otimes 0} = \emptyset$, the empty tensor.

First and second term, Equation 6.2.3a and Equation 6.2.3b: We have

$$\mathcal{S}\left((-1)^b \sum_{i=0}^{a} \tbinom{b-1+i}{i} (\widetilde{\log}(\tfrac{1}{x}))^{a-i} \widetilde{\log}(y)^{b+i} + (-1)^b \sum_{i=0}^{a} \tbinom{b-1+i}{i} (\widetilde{\log}(\tfrac{1}{x}))^{a-i} \operatorname{Li}_{b+i}(y) \right)$$
$$= (-1)^b \sum_{i=0}^{a} \tbinom{b-1+i}{i} (\tfrac{1}{x})^{\otimes a-i} \sqcup\!\sqcup\, y^{\otimes b+i} - (-1)^b \textstyle\sum_{i=0}^{a} \tbinom{b-1+i}{i} (\tfrac{1}{x})^{\otimes a-i} \sqcup\!\sqcup \left((1-y) \otimes y^{\otimes b-1+i}\right)$$
$$= (-1)^b \sum_{i=0}^{a} \tbinom{b-1+i}{i} (\tfrac{1}{x})^{\otimes a-i} \sqcup\!\sqcup \left(\tfrac{y}{1-y} \otimes y^{\otimes b-1+i} \right) .$$

Then we can write $\binom{b-1+i}{i} y^{\otimes b+i-1}$ as $y^{\otimes b-1} \sqcup\!\sqcup\, y^{\otimes i}$, and use the $(-1)^b$ to get

$$= \sum_{i=0}^{a} (\tfrac{1}{x})^{\otimes a-i} \sqcup\!\sqcup \left(\tfrac{1-y}{y} \otimes \left((\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup\, y^{\otimes i} \right) \right) .$$

Sum over the reversed range to get

$$= \sum_{i=0}^{a} (\tfrac{1}{x})^{\otimes i} \sqcup\!\sqcup \left(\tfrac{1-y}{y} \otimes \left((\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup\, y^{\otimes a-i} \right) \right) ,$$

and now apply Lemma 6.2.2 which gives

$$= \sum_{i=0}^{a} \sum_{j=0}^{i} (\tfrac{1}{x})^{\otimes j} \otimes \tfrac{1-y}{y} \otimes \left((\tfrac{1}{x})^{\otimes i-j} \sqcup\!\sqcup\, (\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup\, y^{\otimes a-i} \right) .$$

Interchange the order of summation to get

$$= \sum_{j=0}^{a} \sum_{i=j}^{a} (\tfrac{1}{x})^{\otimes j} \otimes \tfrac{1-y}{y} \otimes \left((\tfrac{1}{x})^{\otimes i-j} \sqcup\!\sqcup\, (\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup\, y^{\otimes a-i} \right) .$$

Finally, use Lemma 6.2.3 to evaluate the inner sum (reindexing to start at $i = 0$), it is

$$= \sum_{j=0}^{a} (\tfrac{1}{x})^{\otimes j} \otimes \tfrac{1-y}{y} \otimes \left((\tfrac{y}{x})^{\otimes a-j} \sqcup\!\sqcup\, (\tfrac{1}{y})^{\otimes b-1} \right)$$
$$= \sum_{i=0}^{a} (\tfrac{1}{x})^{\otimes i} \otimes \tfrac{1-y}{y} \otimes \left((\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup\, (\tfrac{y}{x})^{\otimes a-i} \right)$$

$$= \sum_{i=0}^{a} (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{1}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a-i} \Big) \, .$$

Third term, Equation 6.2.3c: For the third term we have

$$\mathcal{S}\left(-(-1)^a \sum_{i=0}^{b} \binom{a-1+i}{i} (\widetilde{\log}(\tfrac{1}{x}))^{b-i} \operatorname{Li}_{a+i}(\tfrac{x}{y}) \right)$$
$$= (-1)^a \sum_{i=0}^{b} \tbinom{a-1+i}{i} (\tfrac{1}{x})^{\otimes b-i} ⧢ \Big((1 - \tfrac{x}{y}) \otimes (\tfrac{x}{y})^{\otimes a-1+i} \Big) \, .$$

Combine $\binom{a-1+i}{i}$ with $(\frac{x}{y})^{\otimes a-1+i}$, and use the $(-1)^{a-1}$ to get

$$= - \sum_{i=0}^{b} (\tfrac{1}{x})^{\otimes b-i} ⧢ \Big((1 - \tfrac{x}{y}) \otimes \Big((\tfrac{y}{x})^{\otimes a-1} ⧢ (\tfrac{x}{y})^{\otimes i} \Big) \Big)$$
$$= - \sum_{i=0}^{b} (\tfrac{1}{x})^{\otimes i} ⧢ \Big((1 - \tfrac{x}{y}) \otimes \Big((\tfrac{y}{x})^{\otimes a-1} ⧢ (\tfrac{x}{y})^{\otimes b-i} \Big) \Big) \, .$$

Apply Lemma 6.2.2, then reverse the order of summation to get

$$= - \sum_{i=0}^{b} \sum_{j=0}^{i} (\tfrac{1}{x})^{\otimes j} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{x})^{\otimes i-j} ⧢ (\tfrac{y}{x})^{\otimes a-1} ⧢ (\tfrac{x}{y})^{\otimes b-i} \Big)$$
$$= - \sum_{j=0}^{b} \sum_{i=j}^{b} (\tfrac{1}{x})^{\otimes j} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{x})^{\otimes i-j} ⧢ (\tfrac{y}{x})^{\otimes a-1} ⧢ (\tfrac{x}{y})^{\otimes b-i} \Big) \, .$$

Use Lemma 6.2.3 to evaluate the inner sum giving

$$= - \sum_{j=0}^{b} (\tfrac{1}{x})^{\otimes j} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-j} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big)$$
$$= - \sum_{i=0}^{b} (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) \, .$$

Fourth term, Equation 6.2.3d: For the fourth term we get

$$\mathcal{S}((-1)^{a+b} \operatorname{Li}_a(\tfrac{x}{y}) \widetilde{\log}^b(y)) = -(-1)^{a+b} \Big((1 - \tfrac{x}{y}) \otimes (\tfrac{x}{y})^{\otimes a-1} \Big) ⧢ y^{\otimes b} \, .$$

Use the $-(-1)^{a+b} = (-1)^{a-1+b}$ to get

$$= \Big((1 - \tfrac{x}{y}) \otimes (\tfrac{y}{x})^{\otimes a-1} \Big) ⧢ (\tfrac{1}{y})^{\otimes b}$$
$$= (\tfrac{1}{y})^{\otimes b} ⧢ \Big((1 - \tfrac{x}{y}) \otimes (\tfrac{y}{x})^{\otimes a-1} \Big) \, ,$$

since $⧢$ is commutative. Now apply Lemma 6.2.2 to write this as

$$= \sum_{i=0}^{b} (\tfrac{1}{y})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) \, .$$

Fifth term, Equation 6.2.3e: The fifth term is

$$\mathcal{S}((-1)^{a+b} \operatorname{Li}_{a+b}(x))$$

$$= -(-1)^{a+b}(1-x) \otimes x^{\otimes a+b-1}$$
$$= (1-x) \otimes (\tfrac{1}{x})^{\otimes a+b-1} \,,$$

after making use of $-(-1)^{a+b} = (-1)^{a+b-1}$.

6.2.5 Symbol of RHS

Summing up all the terms found above, we can write down the symbol of the right hand side as

$$\mathcal{S}(\text{Equation 6.1.1 RHS}) = \sum_{i=0}^{a} (\tfrac{1}{x})^{\otimes i} \otimes (1-\tfrac{1}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-i} \right) + \tag{6.2.4a}$$
$$- \sum_{i=0}^{b} (\tfrac{1}{x})^{\otimes i} \otimes (1-\tfrac{x}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) + \tag{6.2.4b}$$
$$+ \sum_{i=0}^{b} (\tfrac{1}{y})^{\otimes i} \otimes (1-\tfrac{x}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) + \tag{6.2.4c}$$
$$+ (1-x) \otimes (\tfrac{1}{x})^{\otimes a+b-1} \,. \tag{6.2.4d}$$

6.2.6 Comparing both sides

We will prove that both sides agree by comparing the terms which start with the same given tensor. On the LHS we can only get terms which start with $1-y$, y, $1-x$ or x. On the RHS we can get terms which start with $1-y$, y, $1-x$, x, or $x-y$. Let's deal with each in turn.

6.2.6.1 Factors beginning $(1-y)\otimes$

On the left hand side we get a contribution from Equation 6.2.2a and Equation 6.2.2d. It equals

$$\sum_{i=0}^{b-1} (1-y) \otimes (\tfrac{1}{y})^{\otimes i} \otimes (1-\tfrac{y}{x}) \otimes \left((\tfrac{1}{y})^{\otimes b-1-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) +$$
$$- \sum_{i=0}^{b-1} (1-y) \otimes (\tfrac{1}{y})^{\otimes i} \otimes (1-\tfrac{x}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-1-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) \,.$$

By using the following result in one component of the tensor

$$\otimes\, (1-\tfrac{y}{x}) \otimes \;-\; \otimes\, (1-\tfrac{x}{y}) \otimes \;=\; \otimes\, (\tfrac{x-y}{x}) \otimes \;-\; \otimes\, (\tfrac{x-y}{y}) \otimes$$
$$= \otimes\, (\tfrac{x-y}{x} \tfrac{y}{x-y}) \otimes$$
$$= \otimes\, (\tfrac{y}{x}) \otimes \,,$$

this simplifies to

$$= \sum_{i=0}^{b-1} (1-y) \otimes (\tfrac{1}{y})^{\otimes i} \otimes (\tfrac{y}{x}) \otimes \left((\tfrac{1}{y})^{\otimes b-1-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) \,.$$

On the right hand side we only get a partial contribution from the $i = 0$ term of Equation 6.2.4a. This is

$$(1-y) \otimes \left((\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a} \right)$$

By writing $(\frac{y}{x})^{\otimes a} = (\frac{y}{x}) \otimes (\frac{y}{x})^{\otimes a-1}$, and using Lemma 6.2.2, this is

$$= \sum_{i=0}^{b-1} (1-y) \otimes (\tfrac{1}{y})^{\otimes i} \otimes (\tfrac{y}{x}) \otimes \left((\tfrac{1}{y})^{\otimes b-1-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right)$$

which agrees exactly with the left hand contribution above.

6.2.6.2 Factors beginning $y\otimes$

The left hand contribution comes from Equation 6.2.2a, as

$$\sum_{i=0}^{b-1} (\tfrac{1}{y}) \otimes (\tfrac{1}{y})^{\otimes i} \otimes (1 - \tfrac{y}{x}) \otimes \left((\tfrac{1}{y})^{\otimes b-1-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) .$$

On the right hand side, we get a partial contribution from the $i = 0$ term of Equation 6.2.4a, and the $i = 0$ term of Equation 6.2.4b. We get a partial contribution from the $i = 0$ term of Equation 6.2.4c, and full contributions from the $i \geq 1$ terms of this. Overall this gives

$$\begin{aligned} &(\tfrac{1}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a} \right) + \\ &- (\tfrac{1}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) + \\ &+ (\tfrac{1}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) + \\ &+ \sum_{i=1}^{b} (\tfrac{1}{y})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) . \end{aligned}$$

The middle two terms cancel completely to leave

$$\begin{aligned} = (\tfrac{1}{y}) \otimes &\left((\tfrac{1}{y})^{\otimes b-1} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a} \right) + \\ &+ \sum_{i=1}^{b} (\tfrac{1}{y})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \left((\tfrac{1}{y})^{\otimes b-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) . \end{aligned}$$

Let's take the left hand contribution, and reindex the sum to run from $i = 1$ to b, to get

$$= \sum_{i=1}^{b} (\tfrac{1}{y})^{\otimes i} \otimes (1 - \tfrac{y}{x}) \otimes \left((\tfrac{1}{y})^{\otimes b-i} \sqcup\!\sqcup (\tfrac{y}{x})^{\otimes a-1} \right) .$$

Now write

$$(1 - \tfrac{y}{x})\otimes = (\tfrac{x-y}{x})\otimes = (\tfrac{x-y}{y}\tfrac{y}{x})\otimes = (1 - \tfrac{x}{y}) \otimes + (\tfrac{y}{x}) \otimes \ ,$$

and use this to split the sum up into

$$= \sum_{i=1}^{b} (\tfrac{1}{y})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) + \\ + \sum_{i=1}^{b} (\tfrac{1}{y})^{\otimes i} \otimes (\tfrac{y}{x}) \otimes \Big((\tfrac{1}{y})^{\otimes b-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) \,.$$

Using Lemma 6.2.2, and accounting for the missing $i = 0$ term, we can evaluate the second summation as

$$(\tfrac{1}{y})^{\otimes b} ⧢ \big((\tfrac{y}{x}) \otimes (\tfrac{y}{x})^{\otimes a-1} \big) - (\tfrac{y}{x}) \otimes \Big((\tfrac{1}{y})^{\otimes b} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) \,.$$

Using the iterative definition of the shuffle product, we can see this difference is just

$$= (\tfrac{1}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a} \Big) \,.$$

Thus the total contribution from the left hand side is equal to

$$= \sum_{i=1}^{b} (\tfrac{1}{y})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) + \\ + (\tfrac{1}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a} \Big) \,.$$

This is exactly the right hand contribution above.

6.2.6.3 Factors beginning $(x - y)\otimes$

On the left hand side there are no terms which begin with $(x - y)$.

On the right hand side, we get a partial contribution from the $i = 0$ term of Equation 6.2.4b and the $i = 0$ term of Equation 6.2.4c. This contribution is

$$- (x - y) \otimes \Big((\tfrac{1}{y})^{\otimes b} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) + \\ + (x - y) \otimes \Big((\tfrac{1}{y})^{\otimes b} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) \\ = 0 \,.$$

6.2.6.4 Factors beginning $x\otimes$

On the left hand side there is a partial contribution from Equation 6.2.2b and Equation 6.2.2b. We get

$$- \sum_{i=0}^{b-1} (\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) + \\ + \sum_{i=0}^{a-1} (\tfrac{1}{x}) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{1}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a-1-i} \Big)$$

Whereas on the right hand side, there is a contribution from the $i \geq 1$ terms of Equation 6.2.4a, and the $i \geq 1$ terms of Equation 6.2.4b. We get

$$\sum_{i=1}^{a} (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{1}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a-i} \Big) + \\ - \sum_{i=1}^{b} (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) \, .$$

These are equal by substituting $i = j + 1$ into the right hand contribution.

6.2.6.5 Factors beginning $(1 - x)\otimes$

On the right hand side, the contribution is only from Equation 6.2.4d, and is

$$(1 - x) \otimes (\tfrac{1}{x})^{\otimes a+b-1}$$

On the left hand side we get partial contributions from Equation 6.2.2b and Equation 6.2.2c, and full contributions from Equation 6.2.2e and Equation 6.2.2f. Altogether we get

$$- \sum_{i=0}^{b-1} (1-x) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{x}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) + \\ + \sum_{i=0}^{a-1} (1-x) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{1}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a-1-i} \Big) + \\ + \sum_{i=0}^{b-1} (1-x) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1 - \tfrac{y}{x}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) + \\ - \sum_{i=0}^{a-1} (1-x) \otimes (\tfrac{1}{x})^{\otimes i} \otimes (1 - y) \otimes \Big((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a-1-i} \Big) \, .$$

Using

$$- (1 - \tfrac{x}{y}) \otimes + (1 - \tfrac{y}{x}) \otimes = -(\tfrac{x-y}{y}) \otimes + (\tfrac{x-y}{x}) \otimes = (\tfrac{y}{x-y} \tfrac{x-y}{x}) \otimes = (\tfrac{y}{x}) \otimes \text{ and} \\ (1 - \tfrac{1}{y}) \otimes - (1 - y) \otimes = (\tfrac{1-y}{y}) \otimes - (1-y) \otimes = (\tfrac{1}{y}) \otimes \; ,$$

we can combine the two length a sums, and the two length b sums, and pull out the tensor $(1 - x)$ to get

$$= (1 - x) \otimes \Bigg(\sum_{i=0}^{b-1} (\tfrac{1}{x})^{\otimes i} \otimes (\tfrac{y}{x}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1-i} ⧢ (\tfrac{y}{x})^{\otimes a-1} \Big) + \\ + \sum_{i=0}^{a-1} (\tfrac{1}{x})^{\otimes i} \otimes (\tfrac{1}{y}) \otimes \Big((\tfrac{1}{y})^{\otimes b-1} ⧢ (\tfrac{y}{x})^{\otimes a-1-i} \Big) \Bigg) \, .$$

We will make use of the following proposition to evaluate the left hand contribution.

Proposition 6.2.4. *We have*

$$(\alpha\beta)^{\otimes a+b+1} = \sum_{i=0}^{b} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \big(\alpha^{\otimes b-i} ⧢ \beta^{\otimes a} \big) +$$

$$+\sum_{i=0}^{a}(\alpha\beta)^{\otimes i}\otimes\alpha\otimes\left(\alpha^{\otimes b}\sqcup\beta^{\otimes a-i}\right)$$

If we put $\alpha = \frac{1}{y}$ and $\beta = \frac{y}{x}$, and replace a with $a-1$ and b with $b-1$, we get our desired sum. So the proposition tells us the left hand contribution evaluates to

$$(1-x)\otimes(\tfrac{1}{y}\tfrac{y}{x})^{a-1+b-1+1} = (1-x)\otimes(\tfrac{1}{x})^{\otimes a+b-1}\,.$$

This is exactly the right hand contribution.

6.2.7 End of proof

We've now been through all possible starting tensor factors for the left and right hand sides, and shown the left and right hand sides agree in each case. Thus we conclude the left hand side and right hand side are equal, unconditionally. Hence the identity in Theorem 6.1.2 holds exactly on the level of the symbol, as claimed. □

6.2.8 Proof of the proposition

Before the proof of Theorem 6.1.2 is really complete, we need to prove the proposition we introduced above. It reads

Proposition 6.2.4. *We have*

$$(\alpha\beta)^{\otimes a+b+1} = \sum_{i=0}^{b}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b-i}\sqcup\beta^{\otimes a}\right) + \\ +\sum_{i=0}^{a}(\alpha\beta)^{\otimes i}\otimes\alpha\otimes\left(\alpha^{\otimes b}\sqcup\beta^{\otimes a-i}\right)$$

Proof. We will prove this by induction. For $a=0, b=0$, we get

$$\begin{aligned}&(\alpha\beta)^{\otimes 0}\otimes\beta\otimes(\alpha^{\otimes 0}\sqcup\beta^{\otimes 0}) + (\alpha\beta)^{\otimes 0}\otimes\alpha\otimes(\alpha^{\otimes 0}\sqcup\beta^{\otimes 0})\\ &= (\alpha)\otimes + (\beta)\otimes\\ &= (\alpha\beta)\otimes\\ &= (\alpha\beta)^{\otimes 0+0+1}\,.\end{aligned}$$

So the case $a=0, b=0$ holds.

Now fix $a=0$, and we'll induct along b to get the identity for $a=0$ and all b. Assume the identity holds for $(a,b)=(0,b)$, then for $(0,b+1)$, we find

$$\sum_{i=0}^{b+1}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b+1-i}\sqcup\beta^{\otimes 0}\right) + (\alpha\beta)^{\otimes 0}\otimes\alpha\otimes\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes 0}\right)$$

$$= \sum_{i=0}^{b+1} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b+1-i} \sqcup \emptyset\right) + \alpha \otimes \left(\alpha^{\otimes b+1} \sqcup \emptyset\right)$$
$$= \sum_{i=1}^{b+1} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b+1-i} \sqcup \emptyset\right) + \emptyset \otimes \beta \otimes \left(\alpha^{\otimes b+1-0} \sqcup \emptyset\right) + \alpha \otimes \left(\alpha^{\otimes b+1} \sqcup \emptyset\right)$$
$$= \sum_{i=1}^{b+1} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b+1-i} \sqcup \emptyset\right) + (\alpha\beta) \otimes \left(\alpha^{\otimes b+1} \sqcup \emptyset\right) .$$

Reindex the sum to run from $i = 0$, and we get

$$= \sum_{i=0}^{b} (\alpha\beta)^{\otimes i+1} \otimes \beta \otimes \left(\alpha^{\otimes b-i} \sqcup \beta^{\otimes 0}\right) + (\alpha\beta) \otimes \left(\alpha^{\otimes b+1} \sqcup \emptyset\right)$$
$$= (\alpha\beta) \otimes \left(\sum_{i=0}^{b} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b-i} \sqcup \beta^{\otimes 0}\right) + \left(\alpha^{\otimes b+1} \sqcup \emptyset\right)\right)$$
$$= (\alpha\beta) \otimes \left(\sum_{i=0}^{b} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b-i} \sqcup \beta^{\otimes 0}\right) + \alpha \otimes \left(\alpha^{\otimes b} \sqcup \emptyset\right)\right) .$$

Now the expression in brackets is just the result for $(a, b) = (0, b)$. Using the induction hypothesis, we can evaluate this as

$$= (\alpha\beta) \otimes (\alpha\beta)^{\otimes a+b+1}$$
$$= (\alpha\beta)^{\otimes a+(b+1)+1} .$$

Thus the identity holds for $a = 0$ and for all b.

Now fix b and assume we have the identity for (a, b). We'll induct along a to get the identity for $(a + 1, b)$. Since we have the base case $(0, b)$ for any fixed b, we'll get the identity for all (a, b) and the proposition will have been proved.

We need one lemma before completing this step

Lemma 6.2.5. *We have*

$$\sum_{i=0}^{b} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b-i} \sqcup \beta^{\otimes a+1}\right) + \alpha \otimes \left(\alpha^{\otimes b} \sqcup \beta^{\otimes a+1}\right)$$
$$= (\alpha\beta) \otimes \sum_{i=0}^{b} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b-i} \sqcup \beta^{\otimes a}\right) .$$

Proof. For $b = 0$ we get

$$\sum_{i=0}^{0} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes 0-i} \sqcup \beta^{\otimes a+1}\right) + \alpha \otimes \left(\alpha^{\otimes 0} \sqcup \beta^{\otimes a+1}\right)$$
$$= \beta \otimes \left(\emptyset \sqcup \beta^{\otimes a+1}\right) + \alpha \otimes \left(\emptyset \sqcup \beta^{\otimes a+1}\right)$$
$$= (\alpha\beta) \otimes \beta \otimes \beta^{\otimes a}$$
$$= (\alpha\beta) \otimes \sum_{i=0}^{0} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes 0-i} \sqcup \beta^{\otimes a}\right) ,$$

so the base case holds.

Now assume it's true for b. Then for $b+1$ we get

$$\begin{aligned}
&\sum_{i=0}^{b+1}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b+1-i}\sqcup\beta^{\otimes a+1}\right)+\alpha\otimes\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes a+1}\right)\\
=&\sum_{i=1}^{b+1}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b+1-i}\sqcup\beta^{\otimes a+1}\right)+\\
&+\beta\otimes\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes a+1}\right)+\alpha\otimes\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes a+1}\right).
\end{aligned}$$

Reindex the sum to start from $i=0$, and combine the other two terms in the equation, giving

$$\begin{aligned}
&=(\alpha\beta)\otimes\sum_{i=0}^{b}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b-i}\sqcup\beta^{\otimes a+1}\right)+(\alpha\beta)\otimes\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes a+1}\right)\\
&=(\alpha\beta)\otimes\left(\sum_{i=0}^{b}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b-i}\sqcup\beta^{\otimes a+1}\right)+\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes a+1}\right)\right)\\
&=(\alpha\beta)\otimes\left(\sum_{i=0}^{b}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b-i}\sqcup\beta^{\otimes a+1}\right)+\alpha\otimes\left(\alpha^{\otimes b}\sqcup\beta^{\otimes a+1}\right)+\right.\\
&\qquad\left.+\beta\otimes\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes a}\right)\right).
\end{aligned}$$

Now apply the induction hypothesis to the first two terms of the bracket, and get

$$=(\alpha\beta)\otimes\left((\alpha\beta)\otimes\sum_{i=0}^{b}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b-i}\sqcup\beta^{\otimes a}\right)+\beta\otimes\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes a}\right)\right).$$

Bring the tensor $(\alpha\beta)$ into the sum and reindex it to start from $i=1$. Then observe the remaining term is the $i=0$ term of the new sum, so we get

$$\begin{aligned}
&=(\alpha\beta)\otimes\left(\sum_{i=1}^{b+1}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b+1-i}\sqcup\beta^{\otimes a}\right)+\beta\otimes\left(\alpha^{\otimes b+1}\sqcup\beta^{\otimes a}\right)\right)\\
&=(\alpha\beta)\otimes\left(\sum_{i=0}^{b+1}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b+1-i}\sqcup\beta^{\otimes a}\right)\right).
\end{aligned}$$

This proves the lemma. □

We're now in a position to finish the proof of the proposition. Assume the identity holds for (a,b). Then for $(a+1,b)$ we have

$$\sum_{i=0}^{b}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b-i}\sqcup\beta^{\otimes a+1}\right)+\sum_{i=0}^{a+1}(\alpha\beta)^{\otimes i}\otimes\alpha\otimes\left(\alpha^{\otimes b}\sqcup\beta^{\otimes a+1-i}\right).$$

Pull out the $i=0$ term of the length a sum, and reindex the rest of the that sum to start at $i=0$, giving

$$\begin{aligned}
=&\sum_{i=0}^{b}(\alpha\beta)^{\otimes i}\otimes\beta\otimes\left(\alpha^{\otimes b-i}\sqcup\beta^{\otimes a+1}\right)+\alpha\otimes\left(\alpha^{\otimes b}\sqcup\beta^{\otimes a+1}\right)+\\
&+(\alpha\beta)\otimes\sum_{i=0}^{a}(\alpha\beta)^{\otimes i}\otimes\alpha\otimes\left(\alpha^{\otimes b}\sqcup\beta^{\otimes a-i}\right).
\end{aligned}$$

The previous lemma tells us how we can combine the first two terms, so we find

$$= (\alpha\beta) \otimes \sum_{i=0}^{b} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b-i} \sqcup\!\sqcup \beta^{\otimes a}\right) + (\alpha\beta) \otimes \sum_{i=0}^{a} (\alpha\beta)^{\otimes i} \otimes \alpha \otimes \left(\alpha^{\otimes b} \sqcup\!\sqcup \beta^{\otimes a-i}\right)$$
$$= (\alpha\beta) \otimes \left(\sum_{i=0}^{b} (\alpha\beta)^{\otimes i} \otimes \beta \otimes \left(\alpha^{\otimes b-i} \sqcup\!\sqcup \beta^{\otimes a}\right) + \sum_{i=0}^{a} (\alpha\beta)^{\otimes i} \otimes \alpha \otimes \left(\alpha^{\otimes b} \sqcup\!\sqcup \beta^{\otimes a-i}\right) \right).$$

The induction hypothesis lets us evaluate this to get

$$= (\alpha\beta) \otimes (\alpha\beta)^{\otimes a+b+1}$$
$$= (\alpha\beta)^{\otimes (a+1)+b+1} .$$

This completes the proof of the proposition. □

6.3 Numerically testable version

The result in Theorem 6.1.2 establishes a symbol-level identity relating $I_{a,b}(x, y)$ and $I_{a,b}(\frac{1}{x}, \frac{1}{y})$, including all the leading order polylog terms, and the product terms. Unfortunately for numerical checks this is still not enough, since the symbol does not see terms of the form constant $\times$ lower weight.

Using Brown's setup of the Ihara coaction, successive slices of the MPL coproduct can be calculated. These slices allow one to determine corrections to the identity, adding terms with higher and higher weight constant factors, until one arrives at a genuine numerically testable identity.

In what follows we mimic Duhr's approach from the weight 4 case [Gan16], to arrive at such numerically testable identities at weight 5 for $I_{4,1}(x, y)$, and weight 6 for $I_{5,1}(x, y)$. From there we will extrapolate what a general identity for $I_{n,1}(x, y)$ should look like.

6.3.1 Symbol-level identity for $a = n$, $b = 1$

Firstly, we want to give a slightly different formulation of the identity when $a = n$, and $b = 1$. If we set $a = n$, $b = 1$ in Theorem 6.1.2, we obtain, after some obvious simplification

$$I_{n,1}(x, y) + (-1)^n I_{n,1}(\tfrac{1}{x}, \tfrac{1}{y}) \overset{\mathcal{S}}{=} \tag{6.3.1a}$$
$$- \sum_{i=0}^{n} (\widetilde{\log}(\tfrac{1}{x}))^{n-i}\, \widetilde{\log}(y)^{1+i} + \tag{6.3.1b}$$
$$- \sum_{i=0}^{n} (\widetilde{\log}(\tfrac{1}{x}))^{n-i} \operatorname{Li}_{1+i}(y) + \tag{6.3.1c}$$
$$- (-1)^n \sum_{i=0}^{1} \tbinom{n-1+i}{i} (\widetilde{\log}(\tfrac{1}{x}))^{1-i} \operatorname{Li}_{n+i}(\tfrac{x}{y}) + \tag{6.3.1d}$$
$$- (-1)^n \operatorname{Li}_n(\tfrac{x}{y})\, \widetilde{\log}^{1}(y) - (-1)^n \operatorname{Li}_{n+1}(x) . \tag{6.3.1e}$$

Now consider Equation 6.3.1b. We can rewrite this as follows, to say

$$\begin{aligned}
-\sum_{i=0}^{n}(\widetilde{\log}(\tfrac{1}{x}))^{n-i}\,\widetilde{\log}(y)^{1+i} &= -\sum_{i=0}^{n}\frac{1}{(n-i)!(i+1)!}(\log(\tfrac{1}{x}))^{n-i}\log(y)^{1+i} \\
&= -\frac{1}{(n+1)!}\sum_{i=0}^{n}\tfrac{(n+1)!}{(n-i)!(i+1)!}(\log(\tfrac{1}{x}))^{n-i}\log(y)^{1+i} \\
&= -\tfrac{1}{(n+1)!}\left(-\log(\tfrac{1}{x})^{n+1}+\sum_{i=-1}^{n}\tfrac{(n+1)!}{(n-i)!(i+1)!}(\log(\tfrac{1}{x}))^{n-i}\log(y)^{1+i}\right).
\end{aligned}$$

Substitute $j = i+1$ into the sum. Then we can recognise the result as a binomial expansion, and obtain

$$\begin{aligned}
&= -\frac{1}{(n+1)!}\left(-\log(\tfrac{1}{x})^{n+1}+\sum_{j=0}^{n+1}\tfrac{(n+1)!}{(n+1-j)!j!}(\log(\tfrac{1}{x}))^{n+1-j}\log(y)^{j}\right) \\
&= -\frac{1}{(n+1)!}\left(-\log(\tfrac{1}{x})^{n+1}+(\log(\tfrac{1}{x})+\log(y))^{n+1}\right) \\
&= -\frac{1}{(n+1)!}\left(-\log(\tfrac{1}{x})^{n+1}+\log(\tfrac{y}{x})^{n+1}\right).
\end{aligned}$$

Finally a factor of $-(-1)^n = (-1)^{n+1}$ can be pulled out using $\log(\frac{1}{x}) = -\log(x)$. So the overall result is

$$= (-1)^n\frac{1}{(n+1)!}(\log(\tfrac{x}{y})^{n+1}-\log(x)^{n+1}).$$

For Equation 6.3.1c, we have

$$-\sum_{i=0}^{n}(\widetilde{\log}(\tfrac{1}{x}))^{n-i}\operatorname{Li}_{1+i}(y) = \sum_{i=0}^{n}\tfrac{1}{(n-i)!}(-\log(x))^{n-i}\operatorname{Li}_{1+i}(y)$$

Now set $j = n-i$, so the sum runs from $j = 0$ to $j = n$, but the terms appear in the reverse order. We get

$$= -\sum_{j=0}^{n}\frac{1}{j!}(-\log(x))^{j}\operatorname{Li}_{n+1-j}(y).$$

The sum in Equation 6.3.1d contains simply the following two terms

$$-(-1)^n(\log(\tfrac{1}{x})\operatorname{Li}_n(\tfrac{x}{y})+n\operatorname{Li}_{n+1}(\tfrac{x}{y})).$$

And Equation 6.3.1e is just

$$-(-1)^n\operatorname{Li}_n(\tfrac{x}{y})\log(y)-(-1)^n\operatorname{Li}_{n+1}(x).$$

We can combine the first terms of the previous two lines to get overall

$$-(-1)^n(-\operatorname{Li}_n(\tfrac{x}{y})\log(\tfrac{x}{y})+n\operatorname{Li}_{n+1}(\tfrac{x}{y})+\operatorname{Li}_{n+1}(x)).$$

If we plug these simplifications back into Equation 6.3.1, and take everything over to the left hand side we obtain

$$I_{n,1}(x,y)+(-1)^n I_{n,1}(\tfrac{1}{x},\tfrac{1}{y})+ \tag{6.3.2a}$$

$$+ (-1)^n(-\mathrm{Li}_n(\tfrac{x}{y})\log(\tfrac{x}{y}) + n\,\mathrm{Li}_{n+1}(\tfrac{x}{y}) + \mathrm{Li}_{n+1}(x)) + \tag{6.3.2b}$$

$$+ \sum_{j=0}^{n} \tfrac{1}{j!}(-\log(x))^j\,\mathrm{Li}_{n+1-j}(y) - (-1)^n \frac{1}{(n+1)!}(\log(\tfrac{x}{y})^{n+1} - \log(x)^{n+1}) \overset{\mathcal{S}}{=} 0\,. \tag{6.3.2c}$$

6.3.2 Weight 5 full identity for $I_{4,1}(x,y) + I_{4,1}(\frac{1}{x},\frac{1}{y})$

In the process of computing the coproduct corrections, we need to make simplifications to the resulting symbols. These simplifications come in the form of lower-weight versions of this numerically testable identity.

Firstly, from Equation 6.3.2, setting $n = 4$, we already have the following 'top-level' slice of what will become a numerically testable identity.

$$I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x},\tfrac{1}{y}) + (-\mathrm{Li}_4(\tfrac{x}{y})\log(\tfrac{x}{y}) + 4\,\mathrm{Li}_5(\tfrac{x}{y}) + \mathrm{Li}_5(x)) +$$
$$+ \sum_{j=0}^{4} \tfrac{1}{j!}(-\log(x))^j\,\mathrm{Li}_{5-j}(y) - \frac{1}{5!}(\log(\tfrac{x}{y})^5 - \log(x)^5) \overset{\mathcal{S}}{=} 0$$

Now compute $-\Delta_{11111}$ (so the result is the correction we need to *add*), expand out the logarithms, simplify and convert to symbols. The slice Δ_{11111} of the coproduct can be computed in Mathematica using the `Delta11111` command from Duhr's PolylogTools package [PT], other slices $\Delta_{k11\cdots1}$ can be computed with the command `Deltak1...1`.

For $-\Delta_{11111}$, we get

$$\begin{aligned}
&-\Delta_{11111} = \\
&\mathrm{i}\pi \otimes \Big(-(x\otimes x\otimes x\otimes x) + x\otimes x\otimes x\otimes(1-y) + x\otimes x\otimes(1-y)\otimes x - x\otimes x\otimes(1-y)\otimes y + \\
&+ x\otimes(1-y)\otimes x\otimes x - x\otimes(1-y)\otimes x\otimes y - x\otimes(1-y)\otimes y\otimes x + x\otimes(1-y)\otimes y\otimes y + \\
&+ (1-y)\otimes x\otimes x\otimes x - (1-y)\otimes x\otimes x\otimes y - (1-y)\otimes x\otimes y\otimes x + (1-y)\otimes x\otimes y\otimes y + \\
&- (1-y)\otimes y\otimes x\otimes x + (1-y)\otimes y\otimes x\otimes y + (1-y)\otimes y\otimes y\otimes x - (1-y)\otimes y\otimes y\otimes y\Big)\,.
\end{aligned}$$

This can then be integrated to

$$\begin{aligned}
&\mathrm{i}\pi(-(\tfrac{1}{4!}\log^4(x) + \tfrac{1}{3!}\mathrm{Li}_1(y)\log^3(x) - \tfrac{1}{2!}\mathrm{Li}_2(y)\log^2(x) + \tfrac{1}{1!}\mathrm{Li}_3(y)\log(x) - \tfrac{1}{0!}\mathrm{Li}_4(y))) \\
&= \mathrm{i}\pi\left(-\tfrac{1}{4!}\log^4(x) + \sum_{i=0}^{3}\tfrac{1}{i!}(-\log(x))^i\,\mathrm{Li}_{4-i}(y)\right)\,.
\end{aligned}$$

Now add this correction to the identity, and compute $-\Delta_{2111}$. After simplifying $-\Delta_{2111}$ with the weight 2 version of the identity, and the dilogarithm inversion formula, then converting to symbols we get

$$\begin{aligned}
-\Delta_{2111} =& \frac{\pi^2}{6}\otimes\Big(-4x\otimes x\otimes x + 2x\otimes x\otimes(1-y) + 2x\otimes x\otimes y + 2x\otimes(1-y)\otimes x + \\
&- 2x\otimes(1-y)\otimes y + 2x\otimes y\otimes x - 2x\otimes y\otimes y + 2(1-y)\otimes x\otimes x +
\end{aligned}$$

$$- 2(1-y)\otimes x\otimes y - 2(1-y)\otimes y\otimes x + 2(1-y)\otimes y\otimes y + 2y\otimes x\otimes x +$$
$$\left. - 2y\otimes x\otimes y - 2y\otimes y\otimes x + 2y\otimes y\otimes y\right),$$

which integrates to

$$\frac{-2\pi^2}{6}\left(\tfrac{1}{3!}(\log^3(\tfrac{x}{y}) + \log^3 x) + \sum_{i=0}^{2}\tfrac{1}{i!}(-\log(x))^i \operatorname{Li}_{3-i}(y))\right).$$

Add in this correction, and compute $-\Delta_{311}$. It turns out there is no contribution here. So on to $-\Delta_{41}$, and we find it is

$$-\Delta_{41} = \tfrac{\pi^4}{90}\otimes(-8[x] + 2[1-y] + 6[y]),$$

which integrates to

$$\tfrac{-2\pi^4}{90}(\tfrac{1}{1!}(3\log(\tfrac{x}{y}) + \log(x)) + \sum_{i=0}^{1}\tfrac{1}{i!}(-\log(x))^i \operatorname{Li}_{1-i}(y)).$$

The last step is to compute the weight 5 pure constant term. In this case the term appears to be 0, numerically.

Combining all of these corrections gives us the following claim.

Claim 6.3.1. *The following identity is a numerically testable functional equation for $I_{4,1}$, at weight 5, in two variables.*

$$\begin{aligned}
&I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x},\tfrac{1}{y}) + \\
&\quad + (\operatorname{Li}_5(x) + 4\operatorname{Li}_5(\tfrac{x}{y}) - \log(\tfrac{x}{y})\operatorname{Li}_4(\tfrac{x}{y})) + \\
&\quad \tfrac{1}{5!}(-\log^5(\tfrac{x}{y}) + \log^5(x)) + \sum_{i=0}^{4}\tfrac{1}{i!}(-\log(x))^i\operatorname{Li}_{5-i}(y) + \\
&\quad + i\pi\left(-\tfrac{1}{4!}\log^4(x) + \sum_{i=0}^{3}\tfrac{1}{i!}(-\log(x))^i\operatorname{Li}_{4-i}(y)\right) + \\
&\quad + \tfrac{-2\pi^2}{6}\left(\tfrac{1}{3!}(\log^3(\tfrac{x}{y}) + \log^3(x)) + \sum_{i=0}^{2}\tfrac{1}{i!}(-\log(x))^i\operatorname{Li}_{3-i}(y)\right) + \\
&\quad + \tfrac{-2\pi^4}{90}\left(\tfrac{1}{1!}(3\log(\tfrac{x}{y}) + \log(x)) + \sum_{i=0}^{0}\tfrac{1}{i!}(-\log(x))^i\operatorname{Li}_{1-i}(y)\right) \stackrel{?}{=} 0.
\end{aligned}$$

Evidence. In Mathematica, this combination evaluates to 0 to with at least 10^{-67}, for various choices of x, y. □

6.3.3 Weight 6 full identity for $I_{5,1}(x,y) - I_{5,1}(\frac{1}{x},\frac{1}{y})$

We can do the same thing at weight 6, as follows. When $n = 5$, we obtain the following symbol level identity

$$I_{5,1}(x,y) - I_{5,1}(\tfrac{1}{x},\tfrac{1}{y}) - (-\operatorname{Li}_5(\tfrac{x}{y})\log(\tfrac{x}{y}) + 5\operatorname{Li}_6(\tfrac{x}{y}) + \operatorname{Li}_6(x)) +$$

$$+\sum_{j=0}^{5}\tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{6-j}(y) + \frac{1}{6!}(\log(\tfrac{x}{y})^6 - \log(x)^6) \overset{\mathcal{S}}{=} 0\,.$$

Now compute $-\Delta_{111111}$, and integrate the result to

$$i\pi(\tfrac{1}{5!}\log^5(x) + \sum_{j=0}^{4}\tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{5-j}(y))\,.$$

Add this correction, and then compute $-\Delta_{21111}$. This result integrates to

$$\tfrac{-2\pi^2}{6}(-\tfrac{1}{4!}(\log^4(\tfrac{x}{y}) + \log^4(x)) + \sum_{j=0}^{3}\tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{4-j}(y))\,.$$

There is again no $-\Delta_{3111}$ contribution. But the result of $-\Delta_{411}$ is non-zero. It integrates to

$$\tfrac{-2\pi^4}{90}(-\tfrac{1}{2!}(3\log^2(\tfrac{x}{y}) + \log^2(x)) + \sum_{j=0}^{1}\tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{2-j}(y))\,.$$

There is no $-\Delta_{51}$ contribution. Finally the pure constant numerically seems to be

$$12\zeta(6) = \tfrac{4\pi^6}{315}\,.$$

Combining all of these corrections leads to the following claim.

Claim 6.3.2. *The following is a numerically testable functional equation for $I_{5,1}$, at weight 6, in two variables.*

$$I_{5,1}(x,y) - I_{5,1}(\tfrac{1}{x},\tfrac{1}{y}) + \tag{6.3.3a}$$

$$-(\operatorname{Li}_6(x) + 5\operatorname{Li}_6(\tfrac{x}{y}) - \log(\tfrac{x}{y})\operatorname{Li}_5(\tfrac{x}{y})) + \tag{6.3.3b}$$

$$-\tfrac{1}{6!}(-\log^6(\tfrac{x}{y}) + \log^6(x)) + \sum_{j=0}^{5}\tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{6-j}(y) + \tag{6.3.3c}$$

$$+ i\pi\left(\tfrac{1}{5!}\log(x)^5 + \sum_{j=0}^{4}\tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{5-j}(y)\right) + \tag{6.3.3d}$$

$$+ \tfrac{-2\pi^2}{6}\left(-\tfrac{1}{4!}(\log(\tfrac{x}{y})^4 + \log^4(x)) + \sum_{j=0}^{3}\tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{4-j}(y)\right) + \tag{6.3.3e}$$

$$+ \tfrac{-2\pi^4}{90}\left(-\tfrac{1}{2!}(3\log^2(\tfrac{x}{y}) + \log^2(x)) + \sum_{j=0}^{1}\tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{2-j}(y)\right) + \tag{6.3.3f}$$

$$+ 12\zeta(6) \overset{?}{=} 0\,. \tag{6.3.3g}$$

6.3.4 Patterns, and an arbitrary weight candidate identity

Within these two instances, and the weight 2, 3, 4 cases not explicitly listed, there is enough information to extrapolate a pattern, and give a candidate for an identity which holds at any weight.

For example, as the weight of the constant increases, viewing $i\pi$ to have weight $k = 1$, $\frac{\pi^2}{6}$ to have weight $k = 2$, *et cetera*, the coefficient of $\log(\frac{x}{y})^{n-k}$ increases exactly according to the weight. (Ignore signs and factorials.) For example, in the weight 6 case we have the following

Constant	Weight	Coefficient
1	0	-1
$i\pi$	1	0
$\frac{\pi^2}{6}$	2	1
No weight 3 constant		
$\frac{\pi^4}{90}$	4	3

Tantalisingly, the pure weight 6 constant $12\zeta(6)$, in Equation 6.3.3g can be interpreted as follows.

$$12\zeta(6) = -2\zeta(6)\left(-\frac{1}{0!}(5\log^0(\tfrac{x}{y}) + \log^0(x)) + \sum_{j=0}^{-1} \tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{0-j}(y)\right).$$

Here $\log^0(x)$ is interpreted as 1, and $\sum_{j=0}^{-1}$ is 0 because the sum is empty.

Notice also that the weight 4 constant in Equation 6.3.3e has the form $-2\frac{\pi^4}{90} = -2\zeta(4)$. Similarly, the weight 2 constant in Equation 6.3.3f has the form $-2\frac{\pi^2}{6} = -2\zeta(2)$.

Using the convention that $\zeta(0) = -\frac{1}{2}$, we can write the third line of the weight 6 identity, Equation 6.3.3c, in the following suggestive manner.

$$-2\zeta(0)\left(-\tfrac{1}{6!}(-\log^6(\tfrac{x}{y}) + \log^6(x)) + \sum_{j=0}^{5} \tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{6-j}(y)\right)$$

Make the following definition, to capture the general structure of the terms in the successive slices.

Definition 6.3.3. The function $\ell_\alpha(\beta; x, y)$, for $\alpha \geq 0 \in \mathbb{Z}$, and $\beta \in \mathbb{Z}$ is defined as follows.

$$\ell_\alpha(\beta; x, y) \coloneqq -(-1)^\alpha \tfrac{1}{\alpha!}(\beta \log^\alpha(\tfrac{x}{y}) + \log^\alpha(x)) + \sum_{j=0}^{\alpha-1} \tfrac{1}{j!}(-\log(x))^j \operatorname{Li}_{\alpha-j}(y).$$

Then the weight 5 identity can be re-written as follows

$$\begin{aligned}
&I_{4,1}(x,y) + I_{4,1}(\tfrac{1}{x}, \tfrac{1}{y}) + \\
&\quad + (\operatorname{Li}_5(x) + 4\operatorname{Li}_5(\tfrac{x}{y}) - \log(\tfrac{x}{y})\operatorname{Li}_4(\tfrac{x}{y})) + \\
&\quad + i\pi f_4(0; x, y) + \\
&\quad - 2\zeta(0)\ell_5(-1; x, y) - 2\zeta(2)\ell_3(1; x, y) - 2\zeta(4)\ell_1(3; x, y) \stackrel{?}{=} 0.
\end{aligned}$$

And similarly, the weight 6 identity can be re-written as

$$\begin{aligned}
&I_{5,1}(x,y) - I_{5,1}(\tfrac{1}{x}, \tfrac{1}{y}) + \\
&\quad - (\operatorname{Li}_6(x) + 5\operatorname{Li}_6(\tfrac{x}{y}) - \log(\tfrac{x}{y})\operatorname{Li}_5(\tfrac{x}{y}))
\end{aligned}$$

$$
\begin{aligned}
&+ i\pi f_5(0;x,y) + \\
&- 2\zeta(0)\ell_6(-1;x,y) - 2\zeta(2)\ell_4(1;x,y) + \\
&- 2\zeta(4)\ell_2(3;x,y) - 2\zeta(6)\ell_0(5;x,y) \stackrel{?}{=} 0\,.
\end{aligned}
$$

Expressions of the same form also give the corresponding identities at weight 2, 3, and 4. We therefore propose the following

Conjecture 6.3.4. *The following identity is a numerically testable functional equation for $I_{n,1}$, at weight $n+1$, in two variables.*

$$
\begin{aligned}
&I_{n,1}(x,y) + (-1)^n I_{n,1}(\tfrac{1}{x},\tfrac{1}{y}) + \\
&\quad + (-1)^n(\mathrm{Li}_{n+1}(x) + n\,\mathrm{Li}_{n+1}(\tfrac{x}{y}) - \log(\tfrac{x}{y})\,\mathrm{Li}_n(\tfrac{x}{y})) + \\
&\quad + i\pi f_n(0;x,y) + \\
&\quad - 2\sum_{\substack{j=0 \\ j \text{ even}}}^{n+1} \zeta(j) f_{n+1-j}(j-1;x,y) = 0
\end{aligned}
$$

Evidence. Testing in Mathematica at weight 7 and 8 (so $n=6$ and $n=7$) gives results equal to 0 to within at least 10^{-50} for various choices of x, y.

Testing for a selection of larger n, such as $n = 12, 33, 123$ also gives 0 numerically. □

In generalising Duhr's result in [Gan16], the above result should provide the first numerically testable functional equation for genuine weight $n+1$ multiple polylogarithms, in at least two variables.

6.4 Further work

Depth 2, all $I_{a,b}$: Conjecture 6.3.4 above gives us a numerically testable functional equation for the iterated integral $I_{n,1}(x,y)$. It arises by taking successive slices of the coproduct, to produce corrections of the form constant × lower weight, with the first slice coming from the symbol level identity Theorem 6.1.2 in the case $a = n$, $b = 1$.

Since the symbol level identity Theorem 6.1.2 holds for all choices of a and b, it is conceivable that this identity could form the first level of a general numerically testable functional equation for $I_{a,b}$. Further work with the coproduct in various special cases might suggest such a general identity.

Indeed a recent paper [FTW16] dealing with the reduction of weight 4 MPL's to Li_4 and $\mathrm{Li}_{2,2}$ includes an example of such a functional equation. Equation 6.4 in [FTW16] states

$$
\begin{aligned}
\mathrm{Li}_{2,2}(x,y) = {} & \mathrm{Li}_{2,2}(\tfrac{1}{x},\tfrac{1}{y}) - \mathrm{Li}_4(xy) + 3\left(\mathrm{Li}_4(\tfrac{1}{x}) + \mathrm{Li}_4(y)\right) + \\
& + 2\left(\mathrm{Li}_3(\tfrac{1}{x}) - \mathrm{Li}_3(y)\right)\log(-xy) + \\
& + \mathrm{Li}_2(\tfrac{1}{x})\left(\tfrac{\pi^2}{6} + \tfrac{1}{2}\log^2(-xy)\right) +
\end{aligned}
$$

$$+\tfrac{1}{2}\operatorname{Li}_2(y)\left(\log^2(-xy)-\log^2(-x)\right) .$$

Of course, $\operatorname{Li}_{2,2}(x,y)$ can be re-interpreted as the iterated integral $I_{2,2}(\frac{1}{xy},\frac{1}{y})$. So a change of variables to $x=x'/y$, would give $I_{2,2}(\frac{1}{x'},\frac{1}{y})$, and put this result onto the same footing as the above results.

Higher depth: One is also naturally lead to ask what happens at higher depth, and whether similar numerically testable functional equations can be found.

A small taste of results in this direction comes from the following.

Identity 6.4.1. *The following result holds on the level of the symbol, modulo products, for $n=1,2,3,4$, at least.*

$$\begin{aligned}
&I_{n,1,1}(x,y,z)+(-1)^{n+1+1}I_{n,1,1}(\tfrac{1}{x},\tfrac{1}{y},\tfrac{1}{z}) \overset{\text{ш}}{=} \\
&I_{n,2}(x,y)+(-1)^n I_{n,2}(\tfrac{y}{z},\tfrac{x}{z})+I_{n+1,1}(x,z)+I_{n+1,1}(\tfrac{1}{z},\tfrac{y}{z})+ \\
&\quad -(-1)^n\operatorname{Li}_{n+2}(x)-(-1)^n(n+1)\operatorname{Li}_{n+2}(\tfrac{x}{z})+\operatorname{Li}_{n+2}(z)
\end{aligned}$$

This family might be amenable to an upgrade to a full numerically checkable identity, by computing successive slices of the coproduct.

It appears that explicit symbol-level identities like the above can be found for all depth 3 iterated integrals. For example

Identity 6.4.2. *The following result for $I_{1,3,2}$ holds on the level of the symbol, modulo products.*

$$\begin{aligned}
I_{1,3,2}(x,y,z)+I_{1,3,2}(\tfrac{1}{x},\tfrac{1}{y},\tfrac{1}{z}) &\overset{\text{ш}}{=} -I_{3,3}(\tfrac{y}{x},\tfrac{z}{x})-I_{5,1}(\tfrac{1}{x},\tfrac{y}{x})+ \\
&+I_{4,2}(x,z)-I_{4,2}(\tfrac{1}{y},\tfrac{z}{y})-I_{4,2}(y,z)+I_{4,2}(\tfrac{1}{z},\tfrac{y}{z})+I_{4,2}(z,y)+ \\
&+10\operatorname{Li}_6(\tfrac{x}{z})-10\operatorname{Li}_6(\tfrac{y}{z})-\operatorname{Li}_6(x)-10\operatorname{Li}_6(y)+5\operatorname{Li}_6(z) .
\end{aligned}$$

Remark 6.4.3. It appears that recently, a general result of this form has indeed been proven by Panzer [Pan15] under the name of the *parity theorem* for multiple polylogarithms.

Theorem 6.4.4 (Parity theorem, Theorem 2.5 in [Pan15])**.** *For all indices $(n_1,\ldots,n_d)\in\mathbb{N}^d$, the combination*

$$\operatorname{Li}_{n_1,\ldots,n_d}(z_1,\ldots,z_d)-(-1)^{n_1+\ldots+n_d-d}\operatorname{Li}_{n_1,\ldots,n_d}(\tfrac{1}{z_1},\ldots,\tfrac{1}{z_d})$$

is of depth at most $d-1$.

Panzer says that the depth reduction can be determined explicitly for any indices $(n_1,\ldots,n_d)$. He gives explicit examples of such analytic identities in the depth 2 and depth 3 cases.

Despite subsuming the above $I_{a,b}(x,y)\pm I_{a,b}(\frac{1}{x},\frac{1}{y})$ result, Panzer's proof is of a analytic/differential nature, in contrast with the entirely algebraic proof using symbol and coproduct in Theorem 6.1.2, Claim 6.3.1, and Claim 6.3.2. It could be interesting to compare the two proofs.

Chapter 7

Polylogarithm functional equations from Goncharov-motivated $I_{4,1}$, $I_{5,1}$, $I_{6,1}$ identities

In this chapter we will apply and extend an idea proposed by Goncharov [Gon94] in the weight 4 and and weight 5 cases to find infinite families of functional equations for Li_5 and Li_6. We start by recalling how Goncharov's idea works in the weight 4 case, and mention the results that Gangl found for $I_{3,1}(\text{5-term } \mathrm{Li}_2, z)$ and the resulting Li_4 functional equation ("weight 4" in Section 7.1). Then we recall how Goncharov's idea is supposed to work in the weight 5 case ("weight 5" in Section 7.1), but phrase the approach in terms of the symbol modulo δ.

We will focus mainly on finding Li_n terms for identities arising from $I^{\pm}_{a,b}$ (as in Definition 7.4.1, "symmetrisation") applied to the so-called algebraic Li_2, Li_3, and Li_4 functional equations. To this end, we continue by recalling these algebraic Li_n functional equations (Section 7.3), and set up some notation (Section 7.3.1) to capture the symmetries they force to manifest on the $I^{\pm}_{a,b}$ identities.

We then proceed to find Li_5 terms for $I^{-}_{4,1}(x, \text{algebraic } \mathrm{Li}_2)$ (Theorem 7.4.6) and Li_5 terms for $I^{-}_{4,1}(\text{algebraic } \mathrm{Li}_3, y)$ (Theorem 7.4.11). From these results we derive an family of functional equations for Li_5 (Corollary 7.4.14). We also find Li_5 and Nielsen terms for $I^{-}_{4,1}(\text{3-term } \mathrm{Li}_3, y)$ (Theorem 7.4.17). We combine this with the $I^{-}_{4,1}(x, \text{algebraic } \mathrm{Li}_2 \text{ equation})$ to find another family of functional equations for Li_5 (Corollary 7.4.20), and a reduction for a family of Nielsen terms to Li_5's (Proposition 7.4.19).

Next we generalise this idea to weight 6. We proceed to find Li_6 terms for $I^{+}_{5,1}(\text{algebraic } \mathrm{Li}_3, y)$ (Theorem 7.6.1), and get a family of functional equations for Li_6 (Corollary 7.6.3). We also find Li_6 terms for $I^{-}_{5,1}(\text{algebraic } \mathrm{Li}_4, y)$ (Theorem 7.6.5), and get another family of functional equations for Li_6 (Corollary 7.6.7). Next we find Nielsen and Li_6 terms for $I^{+}_{5,1}(\text{3-term } \mathrm{Li}_3, y)$, and combine this with the algebraic Li_3 equation to get a yet another family of functional equations for Li_6 (Corollary 7.6.13).

We end by offering suggestions for how to maybe push these ideas to weight 7 (Section 7.7), such as considering the further 'symmetrisation' $\widehat{I^{+}_{6,1}}$ with the Li_2 functional equation $\{y\}_2 + \{1-y\}_2$. We find Li_7 terms for $I^{+}_{6,1}(\text{algebraic } \mathrm{Li}_4, y)$ (Theorem 7.7.3), and for $\widehat{I^{-}_{6,1}}(\text{algebraic } \mathrm{Li}_3, y)$ (Theorem 7.7.5). We also find Li_7 and Nielsen terms for $\widehat{I^{-}_{6,1}}(\text{3-term } \mathrm{Li}_3, y)$ (Theorem 7.7.6. Unfortunately, to obtain a family of Li_7 functional equations, we would still need to find a functional equation for $\mathrm{Li}_4(x) + \mathrm{Li}_4(1-x)$. These ideas can also be extended to weight 8 (Section 7.8.1). Finally, we consider how the idea might be pushed to depth 3, to give more *interesting* functional equations in depth 2, starting at weight 6 (Section 7.8.2).

7.1 Introduction

Goncharov [Gon94] suggests an approach to finding highly generic functional equations for Li_4 and Li_5 by understanding (essentially) the depth 2 MPL's $I_{3,1}(x,y)$ and $I_{4,1}(x,y)$. Goncharov's approach is phrased in terms of elements κ and Φ_5, specifically constructed in the Lie coalgebra $\mathcal{L}_\bullet(F)$ and Bloch complex $\mathcal{B}_\bullet(F)$ of (multiple) polylogarithms. Goncharov's definitions of κ and Φ_5 are recalled in Section 7.4.1 below. But the element κ is essentially the symbol of $I_{3,1}$ and the element Φ_5 is essentially the symbol of (a symmetrisation of) $I_{4,1}$. We will prefer to use the symbol approach so the constructions fit better with the narrative of this thesis.

Weight 4: The integral $I_{3,1}(x,y)$ satisfies

$$I_{3,1}(x,y) \overset{\delta}{=} -\{x\}_2 \wedge \{y\}_2 \,.$$

So if one sets $L_2 = \sum a_i[\xi_i] \in \ker \delta_2$ to be a Li_2 functional equation, then one obtains

$$I_{3,1}(L_2, y) = I_{3,1}(\sum a_i[\xi_i], y) \overset{\delta}{=} 0\,.$$

Morally this implies that $I_{3,1}(\sum a_i[\xi_i], y)$ can already be expressed in terms of Li_4's only, modulo products. Similarly by considering another Li_2 functional equation $L_2' = \sum b_i[\zeta_i] \in \ker \delta_2$, one finds that $I_{3,1}(x, L_2') = I_{3,1}(x, \sum b_i[\zeta_i])$ vanishes modulo δ. So one expects the result can be expressed in terms of Li_4's only, modulo products.

By expanding out

$$I_{3,1}(\sum a_i[\xi_i], \sum b_i[\zeta_i])$$

in two ways, one obtains two *different* combinations of Li_4 terms, whose difference is 0 modulo products. This gives a functional equation for Li_4.

The most general functional equation for Li_2, from which all others are expected to follow, is the 5-term relation

$$\sum_i (-1)^i [\mathrm{cr}(x_1, \ldots, \widehat{x_i}, \ldots, x_5)] \in \mathcal{B}_2\,.$$

This makes it the 'best' choice to plug into $I_{3,1}$, to obtain a generic Li_4 equation. This case has been treated by Gangl [Gan16], who has found a 122 term expression for $I_{3,1}(\mathrm{Li}_2 \text{ 5-term}, y)$, and used this to derive a 931 term functional equation for Li_4 in 4 variables.

Earlier work by Gangl [Gan00] found a version of this, and consequently a Li_4 functional equation, by plugging in the so-called *algebraic* Li_2 functional equation

$$\mathrm{Li}_2(\textstyle\sum_i [p_i]) \overset{⧢}{=} 0 \,,$$

where $\{ p_i \} = \{ p_i(t) \}$ are roots of the polynomial $f(t,x) = x^a(1-x)^b - t$, and $a, b \in \mathbb{Z}_{>0}$. This *algebraic* Li_2 functional equation, and the related *algebraic* Li_3 and *algebraic* Li_4 functional equations are explained in more detail in Section 7.3 below.

The version for $I_{3,1}(\text{5-term}, y)$, plugging in the 5-term relation, was only completed relatively recently, after the advent of the symbol of the multiple polylogarithm. The arguments in the Li_4 terms for the 5-term relation are an 'order of magnitude' more complex than those involved in the Li_4 for the *algebraic* Li_2 functional equation, and were only found after much computer experimentation by Gangl.

Weight 5: The integral $I_{4,1}(x,y)$ satisfies

$$I_{4,1}(x,y) \overset{\delta}{=} -\{x\}_2 \wedge \{y\}_3 + \{x\}_3 \wedge \{y\}_2 \;.$$

So if one considers the slight symmetrisations

$$I^{\pm}_{4,1}(x,y) \coloneqq \frac{1}{2}(I_{4,1}(x,y) \pm I_{4,1}(x, \tfrac{1}{y}))\,,$$

one obtains

$$\begin{aligned} I^{+}_{4,1}(x,y) &\overset{\delta}{=} -\{x\}_2 \wedge \{y\}_3 \\ I^{-}_{4,1}(x,y) &\overset{\delta}{=} \{x\}_3 \wedge \{y\}_2 \;. \end{aligned}$$

This isolates the two arguments of $I^{\pm}_{4,1}(x,y)$ to different weight Bloch groups in the sense that in $I^{+}_{4,1}(x,y)$, modulo δ, the variable x only contributes a weight 2 part $\{x\}_2 \in \mathcal{B}_2(F)$ to the weight 5 result in $\mathcal{B}_2(F) \wedge \mathcal{B}_3(F)$, and the variable y only contributes a weight 3 part $\{y\}_3 \in \mathcal{B}_3(F)$ to the weight 5 result in $\mathcal{B}_2(F) \wedge \mathcal{B}_3(F)$. Compare this with the original situation for $I_{4,1}(x,y)$, modulo δ, where the variable x appears simultaneously as $\{x\}_2$ and as $\{x\}_3$, so contributes a weight 2 part, and a weight 3 part to the final result in $\mathcal{B}_2(F) \wedge \mathcal{B}_3(F)$.

Now by appropriately substituting functional equations for Li_2 or for Li_3 into $I^{\pm}_{4,1}(x,y)$, one can guarantee that the result vanishes modulo δ. So morally one expects the result to be expressible in terms of Li_5's only.

To obtain the most generic Li_5 functional equation from this, one wants use the 5-term Li_2 equation, and the 22-term Goncharov Li_3 equation (or preferably the symmetrised 840-term version). So far the 5-term relation appears to remain out of reach: despite allowing thousands of potentially interesting Li_5 (and Nielsen) arguments (generating using Radchenko's sage package MESA [MESA], insight from the weight 4 case, et cetera), I have not yet been able to find an expression for $I^{+}_{4,1}(\text{5-term}, y)$ in terms of Li_5's and Nielsen polylogarithms. We can, however, make some progress by using the algebraic Li_2 and Li_3 equations, as Gangl did originally in the $I_{3,1}$ case [Gan00].

7.2 Overview of results

The table below summarises the identities found in this chapter by plugging Li_n functional equations into iterated integrals $I_{a,b}$.

Weight	Integral	Li_n equation	Where stated	Involves Nielsen?
5	$I_{4,1}^-$	algebraic Li_2	Theorem 7.4.6	
5	$I_{4,1}^-$	algebraic Li_3	Theorem 7.4.11	
5	$I_{4,1}^-$	3-term Li_3	Theorem 7.4.17	✓
6	$I_{5,1}^+$	algebraic Li_3	Theorem 7.6.1	
6	$I_{5,1}^-$	algebraic Li_4	Theorem 7.6.5	
6	$I_{5,1}^+$	3-term Li_3	Theorem 7.6.8	✓
7	$I_{6,1}^+$	algebraic Li_4	Theorem 7.7.3	
7	$\widehat{I_{6,1}^-}$	algebraic Li_3	Theorem 7.7.5	
7	$\widehat{I_{6,1}^-}$	3-term Li_3	Theorem 7.7.6	✓
8	$\widetilde{I_{7,1}^+}$	3-term Li_3	Theorem 7.8.1	✓

Remark 7.2.1. It is curious to note that Nielsen terms only seem to appear when the 3-term Li_3 functional equation is plugged into one of the slots. This table only provides a limited sample of results, so trying to draw firm conclusions from it could potentially be misleading. However, the main structural difference between the 3-term Li_3 functional equation, and the other functional equations above, is the following.

On the level of functions, the 3-term Li_3 functional equation should really be called a 3(+1) term functional equation, in the sense that there is a non-zero constant on the right hand side. We have namely,

$$\mathscr{L}_3(x) + \mathscr{L}_3(1-x) + \mathscr{L}_3(1-\tfrac{1}{x}) = \zeta(3)\,.$$

In the remaining cases, the constant in each of the functional equations is exactly 0.

This table summarises the functional equations found by expanding out $I_{a,b}$ in two different ways using the identities in the above table.

Li_n weight	Integral	Slot 1 of integral	Slot 2 of integral	Where stated
5	$I_{4,1}^-$	algebraic Li_3	algebraic Li_2	Corollary 7.4.14
5	$I_{4,1}^-$	3-term Li_3	algebraic Li_2	Corollary 7.4.20
6	$I_{5,1}^+$	algebraic Li_3	algebraic Li_3	Corollary 7.6.3
6	$I_{5,1}^-$	algebraic Li_4	algebraic Li_4	Corollary 7.6.7
6	$I_{5,1}^+$	algebraic Li_3	3-term Li_3	Corollary 7.6.13

7.3 Algebraic Li_2, Li_3, and Li_4 equations

Let $a, b \in \mathbb{Z}$, and consider the polynomial

$$f(t, x) = x^a (1 - x)^b - t\,. \tag{7.3.1}$$

Let $\{ p_i \} = \{ p_i(t) \}$ be the roots of this equation, so that $f(t, p_i(t)) = 0$. Define c such that $a+b+c = 0$.

Warning 7.3.1. In the following I will assume $a, b > 0$. This means that we have $\prod_j p_j = \pm t$, since t is the constant term in this polynomial, and can use this to rewrite $1 - p_i$ in terms of p_j, as in Equation 7.3.2 below. We also have the identification $\#\text{roots} = a + b = -c$.

Both of these facts will be used extensively in proving Theorem 7.4.6, and in the computer calculations used to establish other identities involving the *algebraic* Li_2, Li_3 and Li_4 equations, namely Theorems 7.4.11, 7.6.1, 7.7.3, 7.7.3 and 7.7.5.

A great deal of work must be expended to identify the coefficients appearing in results for specific values of a, b as a combination of a's, b's, and c's. If the equality $\#\text{roos} = -c$ does not hold (as is the case when $a < 0$, or $b < 0$), we have a fourth variable which can potentially appear in the coefficients, and making the recognition process more onerous.

If we do allow $a > 0$, and any b with $b \notin \{ 0, -a \}$, then Lemma 4.1, Equation (4.1.1), in [Gan95] establishes that

$$\prod_i p_i = \begin{cases} \pm t & \text{if } a + b > 0 \\ \pm 1 & \text{otherwise.} \end{cases}$$

Extending further to the case where $a < 0$ can be achieved simply replacing $t \mapsto 1/t$ in the polynomial f. It is apparent then, that when trying to establish versions of Theorem 7.4.6 for all a, b, a much greater level of care would be needed to deal consistently with the 3 separate cases $\pm 1, \pm t, \pm \frac{1}{t}$ for $\prod_i p_i$.

For the moment restricting to $a, b > 0$ is more than sufficient to produce interesting families of $I_{n,1}$ identities, and families of functional equations for Li_n, and should still provide much insight into the general case in future.

Remark 7.3.2 (Rationally parametrisable case)**.** We should also note that in the case $a = 1, b = 2$, the roots $\{ p_i(t) \}$ can be parametrised by rational functions for a suitable choice of t, as follows. Take

$$t = \frac{(1-y)^2 y^2}{(1 - y + y^2)^3}\,.$$

Then the roots of the equation $f(x, t) = 0$ are given by

$$\begin{aligned} p_1(y) &= \frac{1}{1 - y + y^2} \\ p_2(y) &= \frac{y^2}{1 - y + y^2} \\ p_3(y) &= \frac{(1-y)^2}{1 - y + y^2}\,, \end{aligned}$$

where the set $\{ p_1, p_2, p_3 \}$ is invariant under $y \mapsto 1 - \frac{1}{y}$.

This means that all of the results in this chapter can be given with explicit rational arguments for the case $a = 1, b = 2$, if one desires a concrete example to check. Moreover, the cases $a = -1, b = 3$, and $a = 2, b = -3$ can also be rationally parametrised by substituting $x \mapsto 1 - 1/x$ into the equation $f(x,t) = 0$. This will also give one a way to check explicit cases for $a < 0$ or $b < 0$, as a starting point to a more general analysis for all a, b, in future.

By substituting $x = p_j$ into $f(t,x) = 0$ we obtain

$$1 - p_i = \pm \frac{\prod_i p_i^{1/b}}{p_i^{a/b}} \tag{7.3.2}$$

$$1 - \frac{1}{p_i} = \pm \frac{\prod_i p_i^{1/b}}{p_i^{(a+b)/b}} \,, \tag{7.3.3}$$

up to some b-th root of unity.

Remark 7.3.3. In principle there is a choice of b-th roots to be made above. However, this choice is not relevant to the symbol calculations below, for we have the following equalities on the level of the symbol. If ζ_n is an n-th root of unity, we have

$$\begin{aligned} n(\cdots \otimes \zeta_n x \otimes \cdots) &= \cdots \otimes \zeta_n^n x^n \otimes \cdots \\ &= \cdots \otimes x^n \otimes \cdots \\ &= n(\cdots \otimes x \otimes \cdots) \,, \end{aligned}$$

Dividing by n in the $\mathbb{Q}$-algebra of symbols gives the equality

$$\cdots \otimes \zeta_n x \otimes \cdots = \cdots \otimes x \otimes \cdots \,.$$

We can therefore treat the equalities in Equation 7.3.2 and Equation 7.3.3 as holding exactly, for the purposed of symbol computations.

The following families of algebraic Li_2, Li_3 and Li_4 functional equations are already well known from Gangl [Gan95]. I will, however, include proofs using symbol calculations, because they are short enough to be enlightening without detracting from the story, and they provide something of a template for the proofs of later more complicated identities. These proofs are basically the symbol calculus version of Gangl's original proofs.

Proposition 7.3.4 (Algebraic Li_2 equation, Lemma 4.1, Equation (4.1.4), in [Gan95])**.** *The following is a functional equation for* Li_2*.*

$$\mathrm{Li}_2 \left(\sum_i [p_i] \right) \overset{ш}{=} 0 \,.$$

Proof. Firstly, write $\{x\}_2$ to mean $-(1-x) \wedge x = -(1-x) \otimes x - x \otimes (1-x)$, as usual. Then we compute the symbol, modulo products to be

$$\sum_i \{1-p_i\}_2 = -\sum_i (1-p_i) \wedge p_i \,.$$

Use Equation 7.3.2 to replace the $1-p_i$ term. This gives

$$= -\sum_i \left(\frac{\prod_j p_j^{1/b}}{p_i^{a/b}} \right) \wedge p_i \,.$$

Split up the tensor factor containing the fraction, and pull out the powers, to obtain

$$= -\sum_i \frac{1}{b} \left(\prod_j p_j \right) \wedge p_i + \frac{a}{b} \left(p_i \wedge p_i \right) \,.$$

Since $p_i \wedge p_i = 0$, this simplifies to

$$\begin{aligned} &= -\frac{1}{b} \sum_i \Big(\prod_j p_j \Big) \wedge p_i \\ &= -\frac{1}{b} \Big(\prod_j p_j \Big) \wedge \Big(\prod_j p_j \Big) \\ &= 0 \,. \end{aligned}$$

This proves it is a functional equation for Li_2. ☐

Certain combinations of these arguments, and arguments from the other S_3-orbits, give rise to algebraic functional equations for Li_3 and Li_4 as follows.

Proposition 7.3.5 (Algebraic Li_3 equation, Lemma 4.1, Equation (4.1.5), in [Gan95])**.** *The following is a functional equation for* Li_3.

$$\mathrm{Li}_3 \left(\sum_i -\frac{1}{a}[1-p_i] + \frac{1}{b}[p_i] \right) \overset{\text{ш}}{=} 0 \,.$$

Proof. Since $\{x\}_3 = -(1-x) \wedge x \otimes x = \{x\}_2 \otimes x$, we compute the symbol modulo products to be as follows.

$$\begin{aligned} \sum_i -\frac{1}{a} \{1-p_i\}_3 + \frac{1}{b} \{p_i\}_3 &= \sum_i -\frac{1}{a} \{1-p_i\}_2 \otimes (1-p_i) + \frac{1}{b} \{p_i\}_2 \otimes p_i \\ &= \sum_i \frac{1}{a} \{p_i\}_2 \otimes (1-p_i) + \frac{1}{b} \{p_i\}_2 \otimes p_i \,, \end{aligned}$$

using the functional equation $\{x\}_2 + \{1-x\}_2 = 0$, for Li_2. Now replace $1-p_i$ using Equation 7.3.2. This gives

$$= \sum_i \frac{1}{a} \{p_i\}_2 \otimes \left(\frac{\prod_j p_j^{1/b}}{p_i^{a/b}} \right) + \frac{1}{b} \{p_i\}_2 \otimes p_i \,.$$

Now split up the tensor factor containing the fraction, and pull the powers out, to obtain

$$= \sum_i \frac{1}{ab} \{p_i\}_2 \otimes \Big(\prod_j p_j \Big) - \frac{1}{b} \{p_i\}_2 \otimes p_i + \frac{1}{b} \{p_i\}_2 \otimes p_i$$

$$= \sum_i \frac{1}{ab} \{p_i\}_2 \otimes \Big(\prod_j p_j\Big) .$$

We then get

$$= \frac{1}{ab} \left(\sum_i \{p_i\}_2 \right) \otimes \Big(\prod_j p_j\Big) = 0 ,$$

because Proposition 7.3.4 shows that $\sum_i \{p_i\}_2 = 0$. This proves the initial expression is a functional equation for Li_3. □

Remark 7.3.6. Notice that this functional equation exhibits an anti-symmetry under $a \leftrightarrow b$ and $p_i \leftrightarrow 1 - p_i$. This should manifest in the Li_n terms found in later $I_{4,1}$, $I_{5,1}$, $I_{6,1}$ identities.

Proposition 7.3.7 (Algebraic Li_4 equation, Lemma 4.1, Equation (4.1.6), in [Gan95])**.** *The following is a functional equation for* Li_4*.*

$$\mathrm{Li}_4 \left(\sum_i \frac{1}{a} \left[\frac{1}{1-p_i} \right] + \frac{1}{b} [p_i] + \frac{1}{c} \left[1 - \frac{1}{p_i} \right] \right) \overset{ш}{=} 0 ,$$

where c is defined by $a + b + c = 0$.

Proof. Since $\{x\}_4 = \{x\}_3 \otimes x$, and $\left\{\frac{1}{x}\right\}_4 = -\{x\}_4$,we compute the symbol modulo products to be as follows.

$$\begin{aligned}
&\sum_i \frac{1}{a} \left\{ \frac{1}{1-p_i} \right\}_4 + \frac{1}{b} \{p_i\}_4 + \frac{1}{c} \{1 - 1/p_i\}_4 \\
&= \sum_i \frac{-1}{a} \{1 - p_i\}_4 + \frac{1}{b} \{p_i\}_4 + \frac{1}{c} \{1 - 1/p_i\}_4 \\
&= \sum_i -\frac{1}{a} \{1 - p_i\}_3 \otimes (1 - p_i) + \frac{1}{b} \{p_i\}_3 \otimes p_i + \frac{1}{c} \{1 - 1/p_i\}_3 \otimes (1 - 1/p_i) .
\end{aligned}$$

Now use Equation 7.3.2, and Equation 7.3.3 to replace $1 - p_i$ and $1 - 1/p_j$ in the final tensor factors. We get

$$= \sum_i -\frac{1}{a} \{1 - p_i\}_3 \otimes \left(\frac{\prod_j p_j^{1/b}}{p_i^{a/b}} \right) + \frac{1}{b} \{p_i\}_3 \otimes p_i + \frac{1}{c} \{1 - 1/p_i\}_3 \otimes \left(\frac{\prod_j p_j^{1/b}}{p_i^{(a+b)/b}} \right) .$$

Expand out the fractions and pull down the powers. Since $a + b = -c$, we obtain

$$\begin{aligned}
= \sum_i \bigg(&- \frac{1}{ab} \{1 - p_i\}_3 \otimes \Big(\prod_j p_j\Big) + \frac{1}{bc} \{1 - 1/p_i\}_3 \otimes \Big(\prod_j p_j\Big) + \\
&+ \frac{1}{b} \{1 - p_i\}_3 \otimes p_i + \frac{1}{b} \{p_i\}_3 \otimes p_i + \frac{1}{b} \{1 - 1/p_i\}_3 \otimes p_i \bigg) .
\end{aligned}$$

Recall that

$$\{x\}_3 + \{1 - x\}_3 + \{1 - 1/x\}_3 = 0 , \tag{7.3.4}$$

is a functional equation for Li_3. This means that the second line above vanishes, leaving

$$= \sum_i -\frac{1}{ab} \{1 - p_i\}_3 \otimes \left(\prod_j p_j \right) + \frac{1}{bc} \{1 - 1/p_i\}_3 \otimes \Big(\prod_j p_j\Big)$$

$$= \left(\sum_i -\frac{1}{ab} \{1-p_i\}_3 + \frac{1}{bc} \{1-1/p_i\}_3 \right) \otimes \Big(\prod_j p_j \Big) .$$

Use Equation 7.3.4 to write $\{1-1/p_i\}_3 = -\{p_i\}_3 - \{1-p_i\}_3$, then substitute this in above. We get

$$= \left(\sum_i -\frac{1}{ab} \{1-p_i\}_3 - \frac{1}{bc} \{p_i\}_3 - \frac{1}{bc} \{1-p_i\}_3 \right) \otimes \Big(\prod_j p_j \Big) .$$

Since $c = -a - b$, we have

$$\frac{1}{ab} + \frac{1}{bc} = \frac{1}{b} \frac{a+c}{ac} = \frac{-1}{ac} .$$

So finally the expression simplifies to

$$\begin{aligned} &= \left(\sum_i \frac{1}{ac} \{1-p_i\}_3 - \frac{1}{bc} \{p_i\}_3 \right) \otimes \Big(\prod_j p_j \Big) \\ &= 0 . \end{aligned}$$

This is because the expression in brackets is nothing other than $\frac{1}{c}$ times the Li_3 functional equation from Proposition 7.3.5. This proves the initial expression is a functional equation for Li_4. □

Remark 7.3.8. Notice that this functional equation exhibits a 3-fold symmetry under the cyclic permutation $a \mapsto b \mapsto c$, and $p_i \mapsto 1 - \frac{1}{p_i} \mapsto \frac{1}{1-p_i}$. This should manifest in the Li_n terms found in later $I_{5,1}$, $I_{6,1}$ identities.

Remark 7.3.9. The functional equations in Propositions 7.3.4, 7.3.5 and 7.3.7 hold for any $a, b \in \mathbb{Z}$ with $a > 0$ and $b \notin \{ 0, -a \}$. For further details see Lemma 4.1 in [Gan95].

7.3.1 Some notation for symmetrising Li_n

In order to conveniently describe many of the identities in the following sections, it will be useful to have polynomials whose roots are $p_i, \frac{1}{p_i}, 1-p_i, \ldots$. For that we have the following definition.

Definition 7.3.10 (Polynomials for S_3 action on the roots)**.** The polynomial $g(\alpha, y)$, where α is one of $p, \frac{1}{p}, 1-p, \frac{1}{1-p}, 1-\frac{1}{p}, \frac{p}{p-1}$ is defined by the following table.

α	$g(\alpha, y)$	Roots of $g(\alpha, y) = t$
p	$y^a(1-y)^b$	p_i
$\frac{1}{p}$	$y^c(y-1)^b$	$\frac{1}{p_i}$
$1-p$	$y^b(1-y)^a$	$1-p_i$
$\frac{1}{1-p}$	$y^c(y-1)^a$	$\frac{1}{1-p_i}$
$1-\frac{1}{p}$	$(-y)^b(1-y)^c$	$1-\frac{1}{p_i}$
$\frac{p}{p-1}$	$(-y)^a(y-1)^c$	$\frac{p_i}{p_i-1}$

It will also be useful to have a consistent way of symmetrising Li_n, and its coefficients, using field automorphisms. For that we make the following definition

Definition 7.3.11 (Li_n symmetrisation)**.** Let $\sigma_1, \ldots, \sigma_k$ be automorphisms of some function fields over $\mathbb{C}$. These fields are fields containing the coefficients and arguments of the paticular Li_n's, and we assume initially that each pair of fields is disjoint over $\mathbb{C}$.

By taking the tensor product of these fields, we may assume the domains of the σ_i agree. Let χ_i be a character of $\langle\sigma_i\rangle$. Then we define

$$\mathrm{Li}_n^{\sigma_1,\chi_1;\ldots;\sigma_k,\chi_k}(\alpha[f]) := \mathrm{Li}_n\left(\sum_{g_1\in\langle\sigma_1\rangle}\cdots\sum_{g_k\in\langle\sigma_k\rangle}\chi_1(g_1)\cdots\chi_k(g_k)\alpha^{g_1\cdots g_k}[f^{g_1\cdots g_k}]\right)$$

If the character χ_i is trivial, we may leave it out of the superscript. If the character χ_i acts as -1 on σ_i, we may write σ_i^- in place of σ_i, χ_i.

Remark 7.3.12. By slightly abusing the field automorphism notation, we can let σ first act on the polynomial $g(x,y)$ by $\sigma(g(x,y)) = g(x^\sigma, y^\sigma)$, before evaluating the result.

Example 7.3.13. As an example, suppose we have the field automorphism $r\colon \mathbb{C}(y) \to \mathbb{C}(y)$, defined by $r(y) = \frac{1}{y}$. And $\tau\colon \mathbb{C}(a,b,c,p) \to \mathbb{C}(a,b,c,p)$ defined by $\tau(a) = b$, $\tau(b) = c$, $\tau(c) = a$, and $\tau(p) = 1 - \frac{1}{p}$. Then

$$\begin{aligned}\mathrm{Li}_n^{\tau,r^-}\left(\frac{a}{b}\left[\frac{g(p,y)}{p}y\right]\right) = \mathrm{Li}_n\Bigg(&\frac{a}{b}\left[\frac{g(p,y)}{p}y\right] + \frac{b}{c}\left[\frac{g(1-\frac{1}{p},y)}{1-\frac{1}{p}}y\right] + \frac{c}{a}\left[\frac{g(\frac{1}{1-p},y)}{\frac{1}{1-p}}y\right] + \\ &-\frac{a}{b}\left[\frac{g(p,\frac{1}{y})}{p}\frac{1}{y}\right] - \frac{b}{c}\left[\frac{g(1-\frac{1}{p},\frac{1}{y})}{1-\frac{1}{p}}\frac{1}{y}\right] - \frac{c}{a}\left[\frac{g(\frac{1}{1-p},\frac{1}{y})}{\frac{1}{1-p}}\frac{1}{y}\right]\Bigg).\end{aligned}$$

In this result, each row is generated by the order 3 automorphism σ with trivial character. The columns correspond to applying the order 2 automorphism r with character $\chi_2(r) = -1$.

The table below summarises the automorphisms that will be used throughout the rest of this chapter. It is included as a reference aid since the automorphisms will be introduced as they are needed.

Automorphism	Action	Mnemonic	Where defined
$\rho = \rho_p$	$p \mapsto \frac{1}{p}, a \mapsto c, c \mapsto a$	*reciprocal* of p	Definition 7.4.5
r	$y \mapsto \frac{1}{y}$	*reciprocal* of y	Definition 7.4.8
$\mu = \mu_p$	$a \mapsto b, b \mapsto a, p \mapsto 1-p$	one *minus* p	Definition 7.4.10
ρ_q	$d \mapsto f, f \mapsto d, q \mapsto \frac{1}{q}$		Definition 7.4.13
t	$x \mapsto 1 - \frac{1}{x}$	*three-term* in x	Definition 7.4.16
μ_q	$d \mapsto e, e \mapsto d, q \mapsto 1-q$		Definition 7.6.2
$\tau = \tau_p$	$a \mapsto b \mapsto c \mapsto a, p \mapsto 1 - \frac{1}{p}$	*three-fold* symmetry of p	Definition 7.6.4
τ_q	$d \mapsto e \mapsto f \mapsto d, q \mapsto 1 - \frac{1}{q}$		Definition 7.6.6
s	$y \mapsto 1 - \frac{1}{y}$		Definition 7.6.11
m	$y \mapsto 1-y$	one *minus* y	Definition 7.7.4

7.4 Li_5 functional equations from Goncharov-motivated $I_{4,1}$ identities

As noted in Equation 4.2.8, and Section 4.4.3, the iterated integral $I_{4,1}(x, y)$ satisfies the following

$$I_{4,1}(x, y) \overset{\delta}{=} -\{x\}_2 \wedge \{y\}_3 + \{x\}_3 \wedge \{y\}_2 \,. \tag{7.4.1}$$

Recalling that $\{1/x\}_n = -(-1)^n \{x\}_n$, one can substitute $y \mapsto \frac{1}{y}$ to obtain

$$I_{4,1}(x, \tfrac{1}{y}) \overset{\delta}{=} -\{x\}_2 \wedge \{y\}_3 - \{x\}_3 \wedge \{y\}_2 \,. \tag{7.4.2}$$

Adding or subtracting Equation 7.4.1 and Equation 7.4.2, leads to the following

$$I_{4,1}(x, y) + I_{4,1}(x, \tfrac{1}{y}) \overset{\delta}{=} -2\{x\}_2 \wedge \{y\}_3 \tag{7.4.3}$$

$$I_{4,1}(x, y) - I_{4,1}(x, \tfrac{1}{y}) \overset{\delta}{=} 2\{x\}_3 \wedge \{y\}_2 \,. \tag{7.4.4}$$

We therefore make the following definitions

Definition 7.4.1 ($I^{\pm}_{4,1}$)**.** The *plus* and the *minus symmetrisations* of $I_{4,1}(x, y)$ are defined by

$$\begin{aligned} I^{+}_{4,1}(x, y) &\coloneqq \frac{1}{2}(I_{4,1}(x, y) + I_{4,1}(x, \tfrac{1}{y})) \\ I^{-}_{4,1}(x, y) &\coloneqq \frac{1}{2}(I_{4,1}(x, y) - I_{4,1}(x, \tfrac{1}{y}))\,. \end{aligned}$$

And from Equation 7.4.3 and Equation 7.4.4, we have the following result

Proposition 7.4.2. *Modulo δ, the symmetrisations satisfy*

$$\begin{aligned} I^{+}_{4,1}(x, y) &\overset{\delta}{=} -\{x\}_2 \wedge \{y\}_3 \\ I^{-}_{4,1}(x, y) &\overset{\delta}{=} \{x\}_3 \wedge \{y\}_2 \,. \end{aligned}$$

Notice now that the two variables are 'isolated' and live in different weight tensor factors. That is to say, in the case of $I^{+}_{4,1}(x, y)$ for example, the variable y only appears in the weight 3 Bloch group $\mathcal{B}_3(F)$ as $\{y\}_3$, whereas the variable x only appears in the weight 2 Bloch group $\mathcal{B}_2(F)$ as $\{x\}_2$. Compare this with the original integral $I_{4,1}(x, y)$ where the variable y has a weight 2 contribution $\{y\}_2 \in \mathcal{B}_2(F)$, and a weight 3 contribution $\{y\}_3 \in \mathcal{B}_3(F)$.

Suppose we choose $L_2 = \sum a_i[\xi_i] \in \ker \delta_2$, so that L_2 is a functional equation of Li_2. And we choose $L_3 = \sum b_i[\zeta_i] \in \ker \delta_3$, so that L_3 is a functional equation of Li_3. Then we have

$$I^{+}_{4,1}(L_2, y) \overset{\delta}{=} 0 \text{ and } I^{+}_{4,1}(x, L_3) \overset{\delta}{=} 0\,.$$

So morally we expect to have

$$I^{+}_{4,1}(L_2, y) \overset{ш}{=} \sum_i \alpha_i \,\mathrm{Li}_5(A_i) \text{ and } I^{+}_{4,1}(x, L_3) \overset{ш}{=} \sum_i \beta_i \,\mathrm{Li}_5(B_i)\,,$$

for some arguments A_i and B_i.

Similarly, we have

$$I^{-}_{4,1}(x, L_2) \overset{\delta}{=} 0 \text{ and } I^{-}_{4,1}(L_3, y) \overset{\delta}{=} 0\,.$$

So morally we expect to have

$$I^{-}_{4,1}(x, L_2) \overset{ш}{=} \sum_i \alpha'_i \operatorname{Li}_5(A'_i) \text{ and } I^{-}_{4,1}(L_3, y) \overset{ш}{=} \sum_i \beta'_i \operatorname{Li}_5(B'_i)\,,$$

for some other arguments A'_i and B'_i.

7.4.1 Relation to Goncharov's Φ_5 element

Proposition 7.4.3. *Modulo products, the symbol of $I_{4,1}(x,y)$ be can be expressed as follows.*

$$\begin{aligned} I_{4,1}(x,y) \overset{ш}{=} & \\ & -3\left\{\frac{x}{y}\right\}_5 - \{x\}_5 - \{y\}_5 + \\ & + \left\{\frac{x}{y}\right\}_4 \otimes \frac{1-x}{1-y} + \{x\}_4 \otimes (1-y) + \{y\}_4 \otimes (1-x) + \\ & - \left(\{1-x\}_3 + \{1-y\}_3 - \left\{\frac{1-x}{1-y}\right\}_3 + \left\{\frac{1-1/x}{1-1/y}\right\}_3\right) \otimes \frac{x}{y} \otimes \frac{x}{y} + \\ & + \left(\{x\}_3 \otimes (1-y) - \{y\}_3 \otimes (1-x) + \left\{\frac{x}{y}\right\}_3 \otimes \frac{1-x}{1-y}\right) \otimes \frac{x}{y}\,, \end{aligned}$$

where we write $\{x\}_n$ to mean $-(1-x) \wedge x \otimes x^{n-2}$.

Proof. This is a direct calculation using the Duhr's PolylogTools package [PT] in Mathematica [MA]. Alternatively one could do the tedious computation by hand using the operator $\rho_w = w\Pi_w$ from Section 3.4.1. □

This should be compared with the element $\widetilde{\phi_5}(x,y)$ that Goncharov defines in [Gon94]. This element lives in the dual of the motivic Lie algebra $L(F)_\bullet$, and is defined by

$$\begin{aligned} \widetilde{\phi_5}(x,y) \coloneqq{} & \phi_4\left\{\frac{x}{y}\right\} \otimes \frac{1-x}{1-y} + \phi_4\{x\} \otimes (1-y) + \phi_4\{y\} \otimes (1-x) + \\ & + \phi_4(x,y) \otimes \frac{x}{y} + \\ & - \phi_3\{x\} \otimes \phi_2\{y\} - \phi_3\{y\} \otimes \phi_2\{x\}\,, \end{aligned}$$

According to Goncharov, $\phi_4(x,y)$ is some hypothetical element in the $L(F)^\vee_{-4}$, which satisfies

$$\partial\phi_4(x,y) = \kappa(x,y)\,,$$

where

$$\kappa(x,y) \coloneqq \phi_3\left[-\{1-x\} - \{1-y\} + \left\{\frac{1-x}{1-y}\right\} - \left\{\frac{1-1/x}{1-1/y}\right\}\right] \otimes \frac{x}{y} +$$

$$+ \phi_3\{x\} \otimes (1-y) - \phi_3\{y\} \otimes (1-x) + \phi_3 \left\{\frac{x}{y}\right\} \otimes \frac{1-x}{1-y} +$$
$$- \phi_2\{x\} \wedge \phi_2\{y\} \,.$$

After some informal identifications, there is a very strong resemblance between $\widetilde{\phi_5}(x,y)$, and the symbol of $I_{4,1}(x,y)$ modulo products. The only significant difference comes from the additional Li_5 terms $-3\left\{\frac{x}{y}\right\}_5 - \{x\}_5 - \{y\}_5$ in $I_{4,1}(x,y)$.

This $\widetilde{\phi_5}(x,y)$ is then symmetrised to define the Goncharov's real element of interest, $\Phi_5(x,y)$, as follows.

$$\Phi_5(x,y) \coloneqq \frac{1}{2}\left(\widetilde{\phi_5}(x,y) - \widetilde{\phi_5}(x,\tfrac{1}{y})\right) .$$

This is in much the same way as I symmetrise $I_{4,1}(x,y)$ to obtain $I^-_{4,1}(x,y)$.

7.4.2 Results

The following result means that restricting to one of the symmetrisations $I^+_{4,1}(x,y)$ or $I^-_{4,1}(x,y)$ is sufficient. We do not 'lose' any information from the other one.

Proposition 7.4.4. *Modulo products, the symmetrisations $I^+_{4,1}(x,y)$ and $I^-_{4,1}(x,y)$ can be related as follows.*

$$I^+_{4,1}(x,y) - I^-_{4,1}(y,x) \overset{ш}{=} -2\,\mathrm{Li}_5(xy) - \frac{1}{2}\,\mathrm{Li}_5(x) - \frac{1}{2}\,\mathrm{Li}_5(y)$$

Proof. Writing out the left hand side, we have

$$\frac{1}{2}(I_{4,1}(x,y) + I_{4,1}(x,\tfrac{1}{y})) - \frac{1}{2}(I_{4,1}(y,x) - I_{4,1}(y,\tfrac{1}{x})) \,.$$

From Identity 4.2.4 we know that $I_{4,1}(x,y) \overset{ш}{=} I_{4,1}(y,x)$, so apply this to the third and fourth terms, to get

$$\overset{ш}{=} \frac{1}{2}(I_{4,1}(x,y) + I_{4,1}(x,\tfrac{1}{y})) - \frac{1}{2}(I_{4,1}(x,y) + I_{4,1}(\frac{1}{x}),y)$$
$$\overset{ш}{=} \frac{1}{2}(I_{4,1}(x,\tfrac{1}{y}) - I_{4,1}(\tfrac{1}{x},y)) \,.$$

Now apply Theorem 6.1.2 in the case $a = 4, b = 1$, setting $x \mapsto x$ and $y \mapsto \frac{1}{y}$. One obtains

$$\overset{ш}{=} \frac{1}{2}((-1)^1\tbinom{4+1-1}{4}\,\mathrm{Li}_5(\tfrac{1}{y}) - (-1)^4\tbinom{4+1-1}{1}\,\mathrm{Li}_5(\tfrac{x}{1/y}) + (-1)^5\,\mathrm{Li}_5(x)) \,,$$

which simplified to the result above. □

In certain cases it may be better to use one of the symmetrisations, $I^+_{4,1}(x,y)$ rather than $I^-_{4,1}(x,y)$. This would allow the global symmetry $y \leftrightarrow \frac{1}{y}$ to manifest on the Li_5 terms. But we will end up having to fix one symmetrisation either, $I^-_{4,1}$ or $I^+_{4,1}$, if we want to plug in and *compare* the results of Li_2 and Li_3 functional equations. This means the symmetry $y \leftrightarrow \frac{1}{y}$ will have to break, partly, for one of the equations.

In order to match up better with the Goncharov $\Phi_5(x, y)$ element, I will use the minus symmetrisation $I^-_{4,1}$. This means that the the overall $y \leftrightarrow \frac{1}{y}$ symmetry is obscured when plugging the Li_2 algebraic equation into the second argument. But this symmetry will be manifest when plugging the Li_3 algebraic equation into the first argument.

7.4.2.1 Li_5 terms for $I^-_{4,1}(x, \text{algebraic } \mathrm{Li}_2)$

With some insight from the $I_{3,1}(x, y)$ case [Gan00] in what arguments to choose, and some amount of searching for good arguments using Radchenko's sage package MESA [MESA], I claim the following.

Definition 7.4.5. In what follows $\rho = \rho_p$ will refer to the field automorphism $\rho\colon \mathbb{C}(a, c, p) \to \mathbb{C}(a, c, p)$ defined by $\rho(a) = c$, $\rho(c) = a$, and $\rho(p) = \frac{1}{p}$. And Definition 7.3.11 will be used to define $\mathrm{Li}_n^{\rho^-}$. Here ρ (rho) is a mnemonic for "*reciprocal* of p".

Theorem 7.4.6. *For $I^-_{4,1}$ applied to the Li_2 algebraic equation, we can find explicit Li_5 terms, and give the following identity.*

$$I^-_{4,1}(x, \textstyle\sum_i [p_i]) \overset{\sqcup\!\sqcup}{=}$$

$$-\frac{c}{2}\,\mathrm{Li}_5(x) + b\,\mathrm{Li}_5(1-x) + b\,\mathrm{Li}_5(1-\tfrac{1}{x}) + \tag{7.4.5a}$$

$$+\,\mathrm{Li}_5^{\rho^-}\left(\frac{1}{abc(c-a))}\left[\frac{t}{g(p,x)}\right]\right) + \sum_{p \in \{\, p_i \,\}} \mathrm{Li}_5^{\rho^-}\left(-\frac{b}{8(c-a)}\left[\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right] + \right. \tag{7.4.5b}$$

$$\left. + \left(\frac{c-a}{4b}+1\right)[xp_i] + \frac{b}{a}\left(\left[\frac{1}{1-p_i}\right] - \left[\frac{1-x}{1-p_i}\right] - \left[\frac{1-1/x}{1-p_i}\right]\right)\right) \tag{7.4.5c}$$

Proof. The proof of this identity is a long, intricate (although basically straightforward) calculation using the symbol. Including the proof here would detract from the narrative, and so the proof is relegated to Appendix C. □

Remark 7.4.7. Observe that the left hand side of Theorem 7.4.6 is antisymmetric under $p_i \leftrightarrow \frac{1}{p_i}$. We therefore expect to see this manifest on the right hand side. This is definitely visible to some extent on the RHS, with an interchange $a \leftrightarrow c$. Roughly this is because, if p_i satisfies the equation $x^a(1-x)^b = t$, then $\frac{1}{p_i}$ satisfies the equation $x^c(x-1)^b = t$, or equivalently $x^c(1-x)^b = (-1)^b t$. Be aware however, that using these roots leads to an equation where 'a' < 0, which falls outside the scope of our considerations, and is potentially more problematic for the reasons given in Warning 7.3.1.

Further work to understand these identities for all a, b should lead to a more explicitly symmetrical version. In particular, it should disentangle the coefficients involving c and the coefficients involving the number of roots.

In order to make the potential symmetries more apparent above, it is perhaps better to convert this identity for $I^-_{4,1}$ to the equivalent identity for $I^+_{4,1}$. This can be done as follows.

Definition 7.4.8. In what follows r will refer to the field automorphism $r\colon \mathbb{C}(y) \to \mathbb{C}(y)$ defined by $r(y) = \frac{1}{y}$. In this definition r is a mnemonic for *r*eciprocal of y.

Corollary 7.4.9. *For $I_{4,1}^+$ applied to the* Li_2 *algebraic equation, we can find explicit* Li_5 *terms, and give the following identity.*

$$\begin{aligned}I_{4,1}^+(\sum_i [p_i], y) &\overset{\sqcup\!\sqcup}{=} \mathrm{Li}_5^r\left(\frac{1}{abc(c-a)}\left[\frac{t}{g(p,y)}\right]\right) + \mathrm{Li}_5^r(b[1-y]) + \\ &+ \sum_{p\in\{\,p_i\,\}} \mathrm{Li}_5^r\Bigg(-\frac{b}{8(c-a)}\left[\frac{(1-y)^2p}{y(1-p)^2}\right] + \left(\frac{c-a}{4b}-1\right)[py] - \frac{b}{a}\left[\frac{1-y}{1-p}\right] + \\ &+ \frac{b}{c}\left[\frac{1-y}{1-1/p}\right] - \frac{1}{4}[p] + \frac{b}{2a}\left[\frac{1}{1-p}\right] - \frac{b}{2d}\left[\frac{1}{1-1/p}\right]\Bigg)\end{aligned}$$

Proof. Using Proposition 7.4.4, with $x = p_i$ and summing over i, we have that

$$I_{4,1}^+(\textstyle\sum_i [p_i], y) = I_{4,1}^-(y, \sum_i [p_i]) - \sum_i \left(2\,\mathrm{Li}_5(p_i y) + \frac{1}{2}\,\mathrm{Li}_5(x) + \frac{1}{2}\,\mathrm{Li}_5(p_i)\right) \tag{7.4.6}$$

Using the equivalence $\#\text{roots} = a + b = -c$, we can cancel $-\frac{c}{2}\,\mathrm{Li}_5(x)$ and $-\sum_i \frac{1}{2}\,\mathrm{Li}_5(x)$ in the result. Also the $-\sum_i 2\,\mathrm{Li}_5(p_i y)$ makes the coefficients match in in the $\mathrm{Li}_5(yp_i)$ and $\mathrm{Li}_5(\frac{y}{p_i})$ terms.

Then we can match up the terms which differ by $y \leftrightarrow \frac{1}{y}$ and package them into a Li_5^r. Observe that

$$\frac{(1-1/y)^2}{1/y} = \frac{(1-y)^2}{y}\,,$$

so $\frac{(1-y)^2}{y}$ is invariant under $t \leftrightarrow \frac{1}{y}$. So using this as an argument in Li_5^r gives back the original term with multiplicity 2, and the coefficient only needs to be one-half the original coefficient. A similar observation holds for the p_i term. Also notice that $g(p, y^{-1}) = (1/y)^a(1-1/y)^b = y^c(y-1)^b$. It is now clear that there is an overall $y \leftrightarrow \frac{1}{y}$ symmetry, and so we get the desired result. ☐

7.4.2.2 Li_5 terms for $I_{4,1}^-$(algebraic Li_3, y)

Now let's consider such $I_{4,1}^-$ identities arising from the Li_3 algebraic equation. Since this Li_3 equation has an overall anti-symmetry under $p_i \mapsto 1 - p_i$ and $a \mapsto b$, we should expect this to manifest on the Li_5 terms. Indeed this is the case.

Definition 7.4.10. In what follows $\mu = \mu_p$ is the field automorphism $\mu\colon \mathbb{C}(a,b,p) \to \mathbb{C}(a,b,p)$ defined by $\mu(a) = b$, $\mu(b) = a$, and $\mu(p) = 1-p$. In this μ (mu) is a mnemonic for "one *minus* p".

Also recall the definition of r from Definition 7.4.8.

Theorem 7.4.11. *For $I_{4,1}^-$ applied to the* Li_3 *algebraic equation, we can find explicit* Li_5 *terms, and give the following identity.*

$$I_{4,1}^-\left(\sum_i -\frac{1}{a}[1-p_i] + \frac{1}{b}[p_i], y\right) \overset{\sqcup\!\sqcup}{=} \mathrm{Li}_5^{\mu^-, r^-}\left(\frac{1}{2b(abc)(b-a)}\left[\frac{t}{g(p,y)}\right]\right) + \tag{7.4.7a}$$

$$+ \sum_{p\in\{\,p_i\,\}} \mathrm{Li}_5^{\mu^-, r^-}\left(\frac{1}{8(b-a)}\left[\frac{(1-y)y}{(1-p)p}\right] + \frac{1}{4c}\left[\frac{1-1/y}{1-1/p}\right] - \frac{1}{2b}\left[\frac{p}{1-y}\right] - \frac{a+4b}{2b^2}\left[\frac{p}{y}\right]\right) \tag{7.4.7b}$$

Data. Mathematica verification for (a,b) in $1 \leq a \neq b \leq 7$. $\square$

7.4.2.3 Li_5 functional equation from $I^-_{4,1}$(algebraic Li_3, algebraic Li_2)

In order to obtain the most general possible function equation from these theorems, we should use the roots p_i and q_j of two different polynomials. To that end, make the following definition.

Definition 7.4.12. Let q_j be the roots of $x^d(1-x^e) = u$, where $d, e \in \mathbb{Z}_{>0}$, and set $f = -d-e$. Moreover, define the polynomial $h(\beta, y)$ for $\beta = q, \frac{1}{q}, 1-q, \frac{1}{1-q}, \frac{q}{q-1}, \frac{q-1}{q}$ by analogy with Definition 7.3.10.

The resulting functional equation will retain (for the most part) a $p \leftrightarrow 1-p$, $a \leftrightarrow b$ antisymmetry, and a $q \leftrightarrow \frac{1}{q}$, $d \leftrightarrow f$ antisymmetry. So make the following definition.

Definition 7.4.13. In what follows ρ_q is the field automorphism $\rho_q \colon \mathbb{C}(d,f,q) \to \mathbb{C}(d,f,q)$ defined by $\rho_q(d) = f$, $\rho_q(f) = d$ and $\rho_q(q) = \frac{1}{q}$. This is the q-version of $\rho = \rho_p$ from Definition 7.4.5. We also write μ_p for emphasis that μ is the p-version.

Corollary 7.4.14. *The following functional equation for* Li_5 *is obtained by expanding out the iterated integral* $I^-_{4,1}(\sum_i \frac{-1}{a}[1-p_i] + \frac{1}{b}[p_i], \sum_j [q_j])$ *in two different ways.*

$$
\begin{aligned}
&\sum_{q \in \{q_j\}} \mathrm{Li}_5^{\mu_p^-, \rho_q^-}\left(\frac{-1}{2ab^2c(a-b)}\left[\frac{t}{g(p,q)}\right]\right) + \sum_{p \in \{p_i\}} \mathrm{Li}_5^{\mu_p^-, \rho_q^-}\left(\frac{1}{bdef(d-f)}\left[\frac{u}{h(q,p)}\right]\right) + \\
&+ \sum_{p \in \{p_i\}} \sum_{q \in \{q_i\}} \mathrm{Li}_5^{\mu_p^-, \rho_q^-}\left(\frac{e}{8b(2d+e)}\left[\frac{p(1-q)^2}{(1-p)^2 q}\right] - \frac{db - 4ae - 3be}{4bcf}\left[\frac{p(1-q)}{(1-p)q}\right] + \right. \\
&\qquad \left. - \frac{1}{8(a-b)}\left[\frac{(1-p)p}{(1-q)q}\right] + \frac{bd + 2ae}{2abd}\left[\frac{1-p}{1-q}\right] + \frac{2bd + 2ae + 5be}{4b^2 e}[pq]\right) + \\
&+ \sum_{p \in \{p_i\}} \mathrm{Li}_5^{\mu_p^-}\left(-\frac{ad + ae - 2be}{2ab}[p] - \frac{(a-b)e}{2ab}\left[\frac{p-1}{p}\right]\right) + \sum_{q \in \{q_i\}} \mathrm{Li}_5^{\rho_q^-}\left(-\frac{(a-b)e}{abd}[1-q]\right) \overset{Ш}{=} 0
\end{aligned}
$$

Remark 7.4.15. Unfortunately, I have not yet been able to find the corresponding Li_5 terms for

$$
I^-_{4,1}(x, \text{5-term relation}) \overset{?}{\overset{Ш}{=}} \sum_i \alpha_i \,\mathrm{Li}_5(A_i)\,.
$$

After allowing for potential Nielsen polylogarithms $S_{3,2}(B_i)$, I am still unable to find a reduction

$$
I^-_{4,1}(x, \text{5-term reltaion}) \overset{?}{\overset{Ш}{=}} \sum_i \alpha_i \,\mathrm{Li}_5(A_i) + \sum_j \beta_j S_{3,2}(B_j)\,.
$$

Even for simpler instances, such as the duplication relation, I am currently unable to find Li_5 and/or Nielsen terms.

This situation should perhaps be compared to the situation in weight 4. Gangl gave a reduction of $I_{3,1}(\text{algebraic } \mathrm{Li}_2, y)$ to Li_4 terms in [Gan00]. The reduction of $I_{3,1}(\text{5-term relation}, y)$ to Li_4 terms was finally completed in [Gan16], and the arguments involved are an order of magnitude more complex than the those in the $I_{3,1}(\text{algebraic } \mathrm{Li}_2, y)$ case.

As such, I have thus far been reluctant to try any Li_3 functional equation approaching the complexity of Goncharov's 22-term relation. However I can give an expression for $I_{4,1}^-$ applied to the 3-term Li_3 relation, to show further results are possible.

7.4.2.4 Li_5 and Nielsen terms for $I_{4,1}^-$(3-term Li_3, y)

I can give an expression involving Li_5, and *Nielsen* terms for $I_{4,1}^-$ applied to the 3-term Li_3 equation.

Definition 7.4.16. Let t be the automorphism $t\colon \mathbb{C}(x) \to \mathbb{C}(x)$ defined by $t(x) = 1 - \frac{1}{x}$. Here t is a mneomonic for "*three-term*". Recall r from Definition 7.4.8.

Theorem 7.4.17. *For $I_{4,1}^-$ applied to the 3-term Li_3 functional equation, we can find explicit Li_5 and weight 5 Nielsen terms, and give the following identity.*

$$I_{4,1}^-\left([x] + \left[1 - \frac{1}{x}\right] + \left[\frac{1}{1-x}\right], y\right) \overset{\sqcup\!\sqcup}{=} \tag{7.4.8a}$$

$$\mathrm{Li}_5^{t,r^-}\left(\frac{1}{12}\left[\frac{(1-x)x}{(1-y)y}\right] + [xy] - \frac{1}{4}\left[\frac{1-y}{x}\right] - \frac{1}{4}[x(1-y)] + \frac{1}{6}[1-y]\right) + \tag{7.4.8b}$$

$$-\frac{3}{2}\mathrm{Li}_5(y) + S_{3,2}(y)\,. \tag{7.4.8c}$$

Remark 7.4.18. Notice that all terms except the final two in Equation 7.4.8c exhibit a visible $y \leftrightarrow \frac{1}{y}$ symmetry. The desire to use as few Nielsen polylogarithms as possible breaks the *visible* symmetry, but we do indeed have the $y \leftrightarrow \frac{1}{y}$ symmetry since

$$-\frac{3}{2}\mathrm{Li}_5(y) + S_{3,2}(y) \overset{\sqcup\!\sqcup}{=} \frac{3}{2}\mathrm{Li}_5(\tfrac{1}{y}) - S_{3,2}(\tfrac{1}{y})\,.$$

Heeding this, we could replace the line from Equation 7.4.8c with

$$\frac{1}{2}\left(S_{3,2}(y) - S_{3,2}(\tfrac{1}{y})\right)\,,$$

to give an equivalent identity, which retains the visible symmetry.

7.4.2.5 Li_5 functional equation from $I_{4,1}^-$(3-term Li_3, algebraic Li_2)

We can combine the 3-term Li_3 and the algebraic Li_2 equations to derive a functional equation for Li_5. The resulting functional equation retains a $x \mapsto 1 - \frac{1}{x}$ symmetry, and a (mostly complete) $p_i \leftrightarrow \frac{1}{p_i}$ and $a \leftrightarrow c$ antisymmetry. We can make use of t and ρ_p defined earlier.

Since the 3-term Li_3 functional equation generates weight 5 Nielsen terms in $I_{4,1}^-$, these terms will remain when we expand out $I_{4,1}^-$ in the two different ways. By moving all the Nielsen terms to the LHS and all Li_5 terms to the RHS, we see that the weight 5 Nielsen terms can necessarily be expressed in terms of Li_5. But one expects a simpler combination suffices.

In this case we have the following identity.

Proposition 7.4.19. *Modulo products, the following identity holds.*

$$\sum_{p\in\{\ p_i\ \}} S_{3,2}(p) \overset{\sqcup\!\sqcup}{=} \sum_{p\in\{\ p_i\ \}} \frac{b}{a}\operatorname{Li}_5(1-p) - \frac{a-b}{b}\operatorname{Li}_5(p) + \frac{b}{a+b}\operatorname{Li}_5\left(1-\frac{1}{p}\right) .$$

We can now give the following functional equation for Li_5.

Corollary 7.4.20. *The following functional equation for* Li_5 *is obtained by expanding out the integral* $I^-_{4,1}$ *in two different ways, when it is applied to the 3-term* Li_3 *equation in the first slot, and algebraic* Li_2 *equation in the the second slot.*

$$\begin{aligned}
&\operatorname{Li}_5^{t,\rho_p^-}\left(\frac{-1}{abc(a-c)}\left[\frac{t}{g(p,x)}\right]\right) - \operatorname{Li}_5^t\left(\frac{5c+4a}{2}[x]\right) + \\
&+ \sum_{p\in\{\ p_i\ \}} \operatorname{Li}_5^{t,\rho_p^-}\left(\frac{b}{8(c-a)}\left[\frac{(1-p)^2x}{p(1-x)^2}\right] - \frac{1}{12}\left[\frac{(1-p)p}{(1-x)x}\right] + \frac{5a+4c}{4b}\left[\frac{x}{1-p}\right] + \right.\\
&\left.+ \frac{5a+4c}{4a}[(1-p)x] - \frac{a-c}{4b}[px] + \frac{a-c}{12b}[p] - \frac{5a+4c}{6a}[1-p]\right) \overset{\sqcup\!\sqcup}{=} 0
\end{aligned}$$

Proof. This is obtained by expanding out

$$I^-_{4,1}\left([x] + \left[1-\frac{1}{x}\right] + \left[\frac{1}{1-x}\right], \sum_i [p_i]\right)$$

in two different ways. We can expand out the 3-term Li_3 functional equation in the first slot using Theorem 7.4.17. Or we can expand out the algebraic Li_2 equation in the second slot using Theorem 7.4.6. The difference of these two ways of expanding is now guaranteed to vanish modulo products.

It is possible to convert the particular combination of weight 5 Nielsen terms which appears, into Li_5 terms using the identity from Proposition 7.6.12. Doing so gives the above functional equation. □

7.5 General results on symmetrising $I_{n,1}$

Before continuing to the weight 6 case, it is perhaps useful to state a number of general results about the plus and minus symmetrisations of $I_{n,1}(x,y)$, and how they relate. The ideas from the weight 5 case on what $I_{4,1}(x,y)$ looks like, modulo δ, and on how $I^{\pm}_{4,1}(x,y)$ relate, will occur several more times so having a general result is beneficial.

Firstly, we give the following proposition to establish what $I_{n,1}(x,y)$ looks like, modulo δ.

Proposition 7.5.1. *Modulo* δ*, we have that*

$$I_{n,1}(x,y) \overset{\delta}{=} \sum_{i=2}^{n-1} -(-1)^i \{x\}_i \wedge \{y\}_{n+1-i} .$$

Proof. We will consider the computation of δ from the Lie coalgebra point of view, and then reinterpret the result in terms of symbols. We need to compute the reduced coproduct $\Delta I(0,x,\{0\}^{n-1},y,1)$, but can disregard any product terms, or any terms of weight 1 as we are going to δ.

I claim that the only terms in Δ that contribute to δ are those where the choice of vertices from $V = \{ x, \{0\}^{n-1}, y \}$ (as in the semicircular polygon interpretation Remark 1.2.2) is given by one of the following sets of positions: $\{ 1, 2, 3, \ldots, i \}$, for $2 \leq i \leq n-1$.

First vertex: If the first vertex is at position > 1, then either it occurs at a 0, wherein we get $I(0; \ldots; 0) = 0$, trivially.

$$I(\underbrace{0; x, 0, \ldots, 0}_{\text{trivially } 0}, \ldots, 0, y; 1)$$

Or it occurs at the y, and we get a weight 1 term $I(0, y, 1)$ in the left hand factor of the coproduct because there are no more vertex available to select. That is, we end up with the following vertices in the coproduct:

$$I(0; x, 0, \ldots, 0, \overset{\downarrow}{y}; 1) \rightsquigarrow I(0; y; 1) \otimes I(0; x, \{0\}^n; y) I(y; 1)\,.$$

Therefore the first vertex we select must be position 1 from V.

So we have the following selection of vertices so far (not counting the end points)

$$I(0; \overset{\downarrow}{x}, 0, \ldots, 0, y; 1)\,.$$

Second vertex: Suppose now the second vertex is at position > 2. Where are the remaining vertices? If there are no further vertices, we have a product already and the result vanishes.

$$I(\overset{\downarrow}{0}; \overset{\downarrow}{x}, 0, \ldots, \overset{\downarrow}{0}, \ldots, 0, \ldots, 0, y; \overset{\downarrow}{1}) \rightsquigarrow I(0; x, 0; 1) \otimes I(0; x) I(x; 0, \ldots; 0) I(0; \ldots, y; 1)$$

If there is another vertex, and there is gap between it and the second vertex, then either the integral it describes is trivially 0. Or if this integral is non-zero, we again have a product. Either way the result still vanishes.

$$I(0; \overset{\downarrow}{x}, 0, \ldots, \underbrace{\overset{\downarrow}{0}, \ldots, 0, \ldots, \overset{\downarrow}{0}}_{\text{trivially } 0}, \ldots, 0, y; 1) \rightsquigarrow 0 \text{ or}$$

$$\begin{aligned} &I(0; \overset{\downarrow}{x}, 0, \ldots, \overset{\downarrow}{0}, \ldots, \overset{\downarrow}{0}, \ldots, 0, \overset{\downarrow}{y}; 1) \rightsquigarrow \\ &\quad I(0; x, 0, \ldots, 0, y; 1) \otimes I(0; x) \underbrace{I(x; 0; 0) I(0; 0) \cdots I(0; 0) I(0; \ldots, 0; y)}_{\text{product, so contributes 0 to } \delta \text{ in } \mathcal{L}_\bullet} I(y; 1) \end{aligned}$$

Repeating this argument shows that every position must be selected as vertex, and then we have a weight 1 result, which is ignored.

$$I(0; \overset{\downarrow}{x}, 0, \overset{\downarrow}{0}, \ldots, \overset{\downarrow}{0}, \overset{\downarrow}{y}; 1) \rightsquigarrow I(0; x, 0, \ldots, 0, y; 1) \otimes I(0; x) I(x; 0; 0) I(0; 0) \cdots I(0; 0) I(0; y) I(y; 1)\,.$$

Therefore the second vertex must be place 2 for a non-trivial result.

Subsequence vertices: Suppose that current vertex is labelled by 0, and there are at least two 0's following it. If there is a next vertex, we cannot leave any more gaps: we either select another 0 to get $I(0; \ldots; 0) = 0$. Or we select y and get $I(0; \{0\}^k; y) = I(0, 0; y)^k$, with $k \geq 2$, which is a product.

If there is only one 0 following it, then we cannot select any further vertices otherwise we have a weight 1 result.

This means we always select a sequence of vertices which looks like the following

$$I(0; \overset{\downarrow}{x}, \overset{\downarrow}{0}, \ldots, \overset{\downarrow}{0}, \underbrace{0, \ldots, 0}_{\geq 1 \text{ terms}}, y; 1)\,.$$

This is one of the sets $\{ 1, 2, \ldots, i \}$, with $i \leq n-1$, as claimed above.

Expression for δ: With vertices at positions $\{ 1, 2, \ldots, i \}$ we make the following selection of vertices

$$I(0; \overset{\downarrow}{x}, \underbrace{\overset{\downarrow}{0}, \ldots, \overset{\downarrow}{0}}_{i-1 \text{ terms}}, \underbrace{0, \ldots, 0}_{n-i \text{ terms}}, y; 1)\,.$$

This gives rise to the following term in Δ

$$\begin{aligned} &I(0; x, \{0\}^{i-1}; 1) \otimes I(0; x) I(x; 0) I(0; 0)^{i-2} I(0; \{0\}^{n-i}, y; 1) \\ &= I(0; x, \{0\}^{i-1}; 1) \otimes I(0; \{0\}^{n-i}, y; 1)\,. \end{aligned}$$

Thus we obtain the following expression for $\delta(I_{n,1}(x,y))$

$$\delta(I_{n,1}(x,y)) = \sum_{i=2}^{n-1} I(0; x, \{0\}^{i-1}; 1) \wedge I(0; \{0\}^{n-i}, y; 1)\,.$$

We need to make use of the following regularisation (a version of rule R2 from [Bro12b], given in Equation 1.2.3 in Section 1.2.3.1 above)

$$\begin{aligned} (-1)^{n-i} I(0; \{0\}^{n-i}, \overbrace{y}^{m_1 = 1}; 1) &= \sum_{j_1 = n-i} I(0; y, \{0\}^{m_1 + j_1 - 1}; 1) \\ &= I(0; y, \{0\}^{n-i}; 1)\,. \end{aligned}$$

Doing so means we can write

$$\delta(I_{n,1}(x,y)) = \sum_{i=2}^{n-1} (-1)^{n-i} I(0; x, \{0\}^{i-1}; 1) \wedge I(0; y; \{0\}^{n-i}; 1)\,.$$

Now recognise that $I(0; x, 0^{m-1}; 1) = \mathrm{Li}_m(\frac{1}{x}) \overset{\sqcup\!\sqcup}{=} -(-1)^m \mathrm{Li}_m(x)$, since the factors in δ are taken modulo products. This means δ simplifies to

$$\delta(I_{n,1}(x,y)) = \sum_{i=2}^{n-1} -(-1)^i \mathrm{Li}_i(x) \wedge \mathrm{Li}_{n+1-i}(y)\,.$$

Reinterpreting this on the level of the symbol, using the shorthand $\{x\}_i$ for the symbol of $\mathrm{Li}_i(x)$, modulo products, gives the claimed result. ☐

Then we can define generally the plus and minus symmetrisations of $I_{n,1}$ as follows.

Definition 7.5.2 (Plus, and minus symmetrisations of $I_{n,1}(x,y)$)**.** The *plus* and *minus symmetrisations* of $I_{n,1}(x,y)$ are defined by

$$I^{+}_{n,1}(x,y) \coloneqq \frac{1}{2} \Big(I_{n,1}(x,y) + I_{n,1}(x, \tfrac{1}{y}) \Big)$$

$$I^-_{n,1}(x,y) \coloneqq \frac{1}{2}\Big(I_{n,1}(x,y) - I_{n,1}(x,\tfrac{1}{y})\Big)$$

From Proposition 7.5.1, we can derive how $I^{\pm}_{n,1}(x,y)$ looks modulo δ.

Proposition 7.5.3. *Modulo δ, the symmetrisations satisfy*

$$I^+_{n,1}(x,y) \overset{\delta}{=} -(-1)^n \sum_{\substack{i=2 \\ n+1 \not\equiv i \,(\mathrm{mod}\ 2)}}^{n-1} \{x\}_i \wedge \{y\}_{n+1-i}$$

$$I^-_{n,1}(x,y) \overset{\delta}{=} (-1)^n \sum_{\substack{i=2 \\ n+1 \equiv i \,(\mathrm{mod}\ 2)}}^{n-1} \{x\}_i \wedge \{y\}_{n+1-i} \,.$$

Proof. In forming either of the symmetrisations, we have to invert y. Doing this in the expression for $I_{n,1}(x,y)$, modulo δ, from Proposition 7.5.1, we obtain

$$I_{n,1}(x,\tfrac{1}{y}) \overset{\delta}{=} \sum_{i=2}^{n-1} -(-1)^i \{x\}_i \wedge \left\{\tfrac{1}{y}\right\}_{n+1-i} \,.$$

Use the inversion relation to say

$$\left\{\tfrac{1}{y}\right\}_{n+1-i} = -(-1)^{n+1-i} \{y\}_{n+1-i} \,,$$

and substitute this in to the previous equation to obtain

$$I_{n,1}(x,\tfrac{1}{y}) \overset{\delta}{=} \sum_{i=2}^{n-1} (-1)^{n+1} \{x\}_i \wedge \{y\}_{n+1-i} \,.$$

Notice the signs in $I_{n,1}(x,y)$, modulo δ, alternate, but the signs in $I_{n,1}(x,\frac{1}{y})$ do not. Notice also that the signs of the last term, when $i = n-1$ in both equations, are opposite. In the first it is $-(-1)^i = (-1)^n$, whereas in the second it is $(-1)^{n+1} = -(-1)^n$. Adding the expressions for $I_{n,1}(x,y)$ and $I_{n,1}(x,\frac{1}{y})$ shows that

$$I^+_{n,1}(x,y) = \sum_{i=2}^{n-1} \frac{(-(-1)^i + (-1)^{n+1})}{2} \{x\}_i \wedge \{y\}_{n+1-i} \,.$$

The coefficient $\frac{1}{2}(-(-1)^i + (-1)^{n+1}$ vanishes if $i \equiv n+1 \pmod 2$, and otherwise is $(-1)^{n+1}$, giving

$$I^+_{n,1}(x,y) = -(-1)^n \sum_{\substack{i=2 \\ i \not\equiv n+1 \,(\mathrm{mod}\ 2)}}^{n-1} \{x\}_i \wedge \{y\}_{n+1-i} \,,$$

as claimed.

Subtracting the expression for $I_{n,1}(x,\frac{1}{y})$ from the expression for $I_{n,1}(x,y)$shows that

$$I^-_{n,1}(x,y) = \sum_{i=2}^{n-1} \frac{(-(-1)^i - (-1)^{n+1})}{2} \{x\}_i \wedge \{y\}_{n+1-i} \,.$$

This time the coefficient $\frac{1}{2}(-(-1)^i - (-1)^{n+1})$ vanishes if $i \not\equiv n+1 \pmod 2$, and otherwise is $-(-1)^{n+1}$, giving

$$I^+_{n,1}(x,y) = (-1)^n \sum_{\substack{i=2 \\ i \equiv n+1 \pmod 2}}^{n-1} \{x\}_i \wedge \{y\}_{n+1-i} \,,$$

as also claimed. ☐

Finally, we can relate various combinations of $I^+_{n,1}(x,y), I^-_{n,1}(x,y), I^+_{n,1}(y,x)$ and $I^-_{n,1}(y,x)$ depending on the weight.

Proposition 7.5.4. *When the weight is odd (meaning n is even), we can relate $I^+_{n,1}(x,y)$ and $I^-_{n,1}(x,y)$ as follows.*

$$I^+_{n,1}(x,y) - I^-_{n,1}(y,x) \overset{\text{ш}}{=} -\frac{n}{2} \operatorname{Li}_{n+1}(xy) - \frac{1}{2} \operatorname{Li}_{n+1}(x) - \frac{1}{2} \operatorname{Li}_{n+1}(y) \,.$$

On the other hand, when the weight is even (meaning n is odd), we have the following relations between $I^+_{n,1}(x,y)$ and $I^+_{n,1}(y,x)$, and between $I^-_{n,1}(x,y)$ and $I^-_{n,1}(y,x)$.

$$\begin{aligned} I^+_{n,1}(x,y) + I^+_{n,1}(y,x) &\overset{\text{ш}}{=} \frac{n}{2} \operatorname{Li}_{n+1}(xy) + \frac{1}{2} \operatorname{Li}_{n+1}(x) + \frac{1}{2} \operatorname{Li}_{n+1}(y) \\ &\overset{\text{ш}}{=} -(I^-_{n,1}(x,y) + I^-_{n,1}(y,x)) \,. \end{aligned}$$

Proof. **Odd weight:** The odd weight case is a generalisation of Proposition 7.4.4, as follows. Writing out the left hand side, we have

$$I^+_{n,1}(x,y) - I^-_{n,1}(y,x) = \frac{1}{2}(I_{n,1}(x,y) + I_{n,1}(x, \tfrac{1}{y})) - \frac{1}{2}(I_{n,1}(y,x) - I_{n,1}(y, \tfrac{1}{x})) \,.$$

Since n is even, we know from from Proposition 4.2.5 that $I_{n,1}(x,y) \overset{\text{ш}}{=} I_{n,1}(y,x)$, so apply this to the third and fourth terms, to get

$$\begin{aligned} &\overset{\text{ш}}{=} \frac{1}{2}(I_{n,1}(x,y) + I_{n,1}(x, \tfrac{1}{y})) - \frac{1}{2}(I_{n,1}(x,y) + I_{n,1}(\frac{1}{x}), y) \\ &\overset{\text{ш}}{=} \frac{1}{2}(I_{n,1}(x, \tfrac{1}{y}) - I_{n,1}(\tfrac{1}{x}, y)) \,. \end{aligned}$$

Now apply Theorem 6.1.2 in the case $a = n, b = 1$ (notice n is even), setting $x \mapsto x$ and $y \mapsto \frac{1}{y}$. One obtains

$$\overset{\text{ш}}{=} \frac{1}{2}((-1)^1 \tbinom{n+1-1}{n} \operatorname{Li}_{n+1}(\tfrac{1}{y}) - (-1)^n \tbinom{n+1-1}{1} \operatorname{Li}_{n+1}(\tfrac{x}{1/y}) + (-1)^{n+1} \operatorname{Li}_n(x)) \,,$$

which simplified to the result above.

Even weight: The even weight case is only a slight modification of this. First we deal with the claim that

$$I^+_{n,1}(x,y) + I^+_{n,1}(y,x) \overset{\text{ш}}{=} -(I^-_{n,1}(x,y) + I^-_{n,1}(y,x)) \,.$$

Indeed, we have

$$(I^+_{n,1}(x,y) + I^+_{n,1}(y,x)) + (I^-_{n,1}(x,y) + I^-_{n,1}(y,x)) = I_{n,1}(x,y) + I_{n,1}(y,x) \,,$$

by regrouping the terms, first with third, and second with fourth. Then by Proposition 4.2.5, this vanishes modulo products, since n odd means $-(-1)^n = 1$.

Now how can we write these in terms of polylogs? Writing out the left hand side of the purported identity gives

$$I_{n,1}^+(x,y) + I_{n,1}^+(y,x) = \frac{1}{2}(I_{n,1}(x,y) + I_{n,1}(x,\tfrac{1}{y})) + \frac{1}{2}(I_{n,1}(y,x) + I_{n,1}(y,\tfrac{1}{x}))\,.$$

Since n is odd, we know from Proposition 4.2.5 that $I_{n,1}(x,y) \overset{\sqcup\!\sqcup}{=} -I_{n,1}(y,x)$, so apply this to the third and fourth terms, to get

$$\begin{aligned} &\overset{\sqcup\!\sqcup}{=} \frac{1}{2}(I_{n,1}(x,y) + I_{n,1}(x,\tfrac{1}{y})) - \frac{1}{2}(I_{n,1}(x,y) + I_{n,1}(\tfrac{1}{x},y)) \\ &\qquad \overset{\sqcup\!\sqcup}{=} \frac{1}{2}(I_{n,1}(x,\frac{1}{y}) + I_{n,1}(\tfrac{1}{x},y))\,. \end{aligned}$$

Now apply Theorem 6.1.2 in the case $a = n, b = 1$ (notice n is odd), setting $x \mapsto x$ and $y \mapsto \frac{1}{y}$. One obtains

$$\overset{\sqcup\!\sqcup}{=} \frac{1}{2}((-1)^1\tbinom{n+1-1}{n}\mathrm{Li}_{n+1}(\tfrac{1}{y}) - (-1)^n\tbinom{n+1-1}{1}\mathrm{Li}_{n+1}(\tfrac{x}{1/y}) + (-1)^{n+1}\mathrm{Li}_n(x))\,,$$

which simplified to the result above. □

7.6 Li_6 functional equations from Goncharov-motivated $I_{5,1}$ identities

Goncharov only describes how to obtain identities for Li_4 and Li_5 from such considerations. However, the idea can still be made to work, at least in weight 6.

From Proposition 7.5.1, the iterated integral $I_{5,1}(x,y)$ satisfies

$$I_{5,1}(x,y) \overset{\delta}{=} -\{x\}_2 \wedge \{y\}_4 + \{x\}_3 \wedge \{y\}_3 - \{x\}_4 \wedge \{y\}_2\,.$$

Consider the plus and minus symmetrisations from Definition 7.5.2. From Proposition 7.5.3 we find that, modulo δ, the symmetrisations satisfy

$$\begin{aligned} I_{5,1}^+(x,y) &\overset{\delta}{=} \{x\}_3 \wedge \{y\}_3 \\ I_{5,1}^-(x,y) &\overset{\delta}{=} -\{x\}_2 \wedge \{y\}_4 - \{x\}_4 \wedge \{y\}_2\,. \end{aligned}$$

Therefore, if $L_3 = \sum a_i[\xi_i] \in \ker \delta_3$ is a Li_3 functional equation, plugging L_3 into either argument of $I_{5,1}^+(x,y)$ gives 0 modulo δ. So we morally expect to be able to write

$$\begin{aligned} I_{5,1}^+(L_3,y) &= \sum_i \alpha_i \,\mathrm{Li}_6(A_i) \\ I_{5,1}^+(x,L_3) &= \sum_i \beta_i \,\mathrm{Li}_6(B_i)\,, \end{aligned}$$

for some arguments A_i, B_i. Notice though, that the story is no longer quite so simple for $I^-_{5,1}$, since x appears as both $\{x\}_2$ and $\{x\}_4$. We will consider in Section 7.6.3 how one can proceed in this case.

Moreover, from Proposition 7.5.4 we have the following relations

$$I^+_{5,1}(x,y) + I^+_{5,1}(y,x) \overset{ш}{=} \frac{5}{2}\,\mathrm{Li}_6(xy) + \frac{1}{2}\,\mathrm{Li}_6(x) + \frac{1}{2}\,\mathrm{Li}_6(y)$$
$$I^-_{5,1}(x,y) + I^-_{5,1}(y,x) \overset{ш}{=} -\frac{5}{2}\,\mathrm{Li}_6(xy) - \frac{1}{2}\,\mathrm{Li}_6(x) - \frac{1}{2}\,\mathrm{Li}_6(y)$$

This means that plugging a functional equation into one of the slots of $I^+_{5,1}$ is sufficient. We can derive the result for the other slot automatically. Similarly, plugging something into one of the slots of $I^-_{5,1}$ is also sufficient because we can derive the corresponding result for the other slot automatically.

7.6.1 Li_6 terms for $I^+_{5,1}$(algebraic Li_3, y)

We can find Li_6 terms for $I^+_{5,1}$ applied to the algebraic Li_3 equation. Recalling $\mu = \mu_p$ from Definition 7.4.10, and r from Definition 7.4.8, we have the following.

Theorem 7.6.1. *For* $I^+_{5,1}$ *applied to the* Li_3 *algebraic equation, we can find explicit* Li_6 *terms, and give the following identity.*

$$I^+_{5,1}\left(\sum_i -\frac{1}{a}[1-p_i] + \frac{1}{b}[p_i], y\right) \overset{ш}{=} \mathrm{Li}_6^{\mu^-,r}\left(\frac{-1}{b(abc)(b-a)(2a+b)}\left[\frac{t}{g(p,y)}\right]\right) + \quad (7.6.1a)$$

$$+\sum_{p\in\{\,p_i\,\}} \mathrm{Li}_6^{\mu^-,r}\left(\frac{1}{12(b-a)}\left[\frac{(1-y)y}{(1-p)p}\right] - \frac{1}{24(2a+b)}\left[\frac{p(1-y)^2}{(1-p)^2y}\right] - \frac{1}{2c}\left[\frac{1-1/y}{1-1/p}\right] + \right. \quad (7.6.1b)$$

$$\left. + \frac{1}{b}\left[\frac{p}{1-y}\right] + \frac{2a+9b}{4b^2}\left[\frac{p}{y}\right] - \frac{1}{4a}\left[\frac{1}{1-p}\right] - \frac{1}{4c}\left[1-\frac{1}{p}\right]\right) \quad (7.6.1c)$$

Data. Mathematica verification for (a,b) in $1 \le a \ne b \le 5$. □

7.6.2 Li_6 functional equation from $I^+_{5,1}$(algebraic Li_3, algebraic Li_3)

We can immediately find the corresponding Li_6 terms for $I^+_{5,1}$ applied to the Li_3 algebraic equation in the other slot. The resulting functional equation retains an antisymemtry under $p \leftrightarrow 1-p$, $a \leftrightarrow b$, and under $q \leftrightarrow 1-q$, $d \leftrightarrow e$. So make the following definition

Definition 7.6.2. The automorphism $\mu_q\colon \mathbb{C}(d,e,q) \to \mathbb{C}(d,e,f)$ is defined by $\mu_q(d) = e$, $\mu_q(e) = d$ and $\mu_q(q) = 1-q$. This is the q-version of μ from Definition 7.4.10.

Now we have the following corollary

Corollary 7.6.3. *The following functional equation for* Li_6 *is obtained by expanding out the iterated integral* $I^+_{5,1}(\sum_i \frac{1}{a}[1-p_i] + \frac{1}{b}[p_i], \sum_j \frac{1}{d}[1-q_j] + \frac{1}{e}[q_j])$ *in two different ways.*

$$\sum_{q\in\{\,q_j\,\}} \mathrm{Li}_6^{\mu_p^-,\mu_q^-}\left(\frac{-1}{a^2bc(a-b)(b-c)d}\left[\frac{t}{g(p,q)}\right] + \frac{1}{ab^2c(a-b)(a-c)e}\left[\frac{t}{g(\frac{1}{p},q)}\right]\right) +$$

$$+\sum_{p\in\{\,p_i\,\}} \mathrm{Li}_6^{\mu_p^-,\mu_q^-}\left(\frac{1}{bde^2f(d-e)(d-f)}\left[\frac{u}{h(q,p)}\right]+\frac{1}{bde^2f(d-e)(d-f)}\left[\frac{u}{h(\frac{1}{q},p)}\right]\right)+$$
$$+\sum_{p\in\{\,p_i\,\}}\sum_{q\in\{\,q_i\,\}} \mathrm{Li}_6^{\mu_p^-,\mu_q^-}\left(\frac{(ae-bd)(ad-be)}{24ab(a-b)de(d-e)}\left[\frac{(1-p)p}{(1-q)q}\right]+\frac{(ae-db)(ad+be)}{4abcdef}\left[\frac{p(1-q)}{(1-p)q}\right]+\right.$$
$$+\frac{ae-db}{6b(a-c)e(d-f)}\left[\frac{p(1-q)^2}{(1-p)^2q}\right]-\frac{1}{12b(d-e)}\left[\frac{p-1}{p^2(1-q)q}\right]-\frac{1}{12(a-b)e}\left[\frac{q-1}{(1-p)pq^2}\right]+$$
$$+\frac{bd+2ce}{2bcde}\left[\frac{p-1}{p(1-q)}\right]-\frac{bd+2af}{2abdf}\left[\frac{p(q-1)}{q}\right]+\frac{(ae-bd)(ad-2be)}{2ab^2de^2}\left[\frac{p}{q}\right]+\frac{bd+ae+4be}{2b^2e^2}[pq]+$$
$$\left.-\frac{a-b}{2abe}[q]-\frac{a-b}{4abf}\left[\frac{q-1}{q}\right]-\frac{d-e}{2bde}[p]-\frac{d-e}{4cde}\left[\frac{p-1}{p}\right]\right)\overset{\sqcup\!\sqcup}{=}0$$

7.6.3 Li_6 terms for $I^-_{5,1}$(algebraic Li_4, y)

Also notice that we can do something with the other symmetrisation, using the algebraic Li_4 equation. This Li_4 functional equation is a linear combination of several Li_2 functional equations, so remains a Li_2 functional equation. One might want to refer to it as a $\mathrm{Li}_2+\mathrm{Li}_4$ functional equation. Plugging this algebraic Li_4 functional equation into either slot of $I^-_{5,1}(x,y)$, gives 0 modulo δ. We therefore expect to write the result as Li_6 terms.

Moreover, the algebraic Li_4 equation is symmetric under $b\mapsto c\mapsto a$, and $p_i\mapsto 1-\frac{1}{p_i}\mapsto\frac{1}{1-p_i}$, so we expect this symmetry to be reflected in the Li_6 terms. This does for the most part hold, but problems again occur because (for example) $\frac{1}{1-p_i}$ is a root of $x^c(1-x)^a=(-1)^a t$, so that this equation has 'a' <0. Again, this is outside the current considerations, and is potentially more problematic for the reasons given in Warning 7.3.1. Nevertheless, we have the following.

Definition 7.6.4. The field automorphism $\tau=\tau_p$, is defined by $\tau\colon\mathbb{C}(a,b,c,p)\to\mathbb{C}(a,b,c,p)$ where $a^\tau=b$, $b^\tau=c$, $c^\tau=a$ and $p^\tau=1-\frac{1}{p}$. In this definition τ (tau) is a mnemonic for the "*three-fold* symmerisation" that occurs in the Li_4 algebraic equation.

Also recall r from Definition 7.4.8.

Theorem 7.6.5. *For $I^-_{5,1}$ applied to the Li_4 algebraic equation we can find explicit Li_6 terms, and give the following identity.*

$$I^-_{5,1}\left(\frac{1}{a}\left[\frac{1}{1-p_i}\right]+\frac{1}{b}[p_i]+\frac{1}{c}\left[1-\frac{1}{p_i}\right],y\right)\overset{\sqcup\!\sqcup}{=}\mathrm{Li}_6^{\tau,r^-}\left(\frac{1}{2ab^2d(a-b)(a+2b)}\left[\frac{t}{g(p,y)}\right]\right)+ \tag{7.6.2}$$
$$+\left(1-\frac{b^2}{ac}\right)\mathrm{Li}_6(y)+\sum_{p\in\{\,p_i\,\}}\mathrm{Li}_6^{\tau,r^-}\left(-\frac{1}{12(a-b)}\left[\frac{(1-y)y}{(1-p)p}\right]+\right. \tag{7.6.3}$$
$$\left.-\frac{a+3b}{2b^2}[py]+\frac{1}{4b}\left[\frac{p}{1-y}\right]+\frac{1}{4b}[p(1-y)]\right) \tag{7.6.4}$$

Data. Mathematica verification for (a,b) in $1\le a\ne b\le 5$. □

7.6.4 Li_6 functional equation from $I^-_{5,1}$(algebraic Li_4, algebraic Li_4)

We can immediately find the corresponding Li_6 terms for $I^-_{5,1}$ applied to the Li_4 algebraic equation in the other slot, and use this to find a Li_6 functional equation. This functional equation retains (mostly) a 3-fold symmetry under $p \mapsto 1 - \frac{1}{q}$, with $a \mapsto b \mapsto c \mapsto a$, and a 3-fold symmetry under $q \mapsto 1 - \frac{1}{q}$, with $d \mapsto e \mapsto f \mapsto d$. To capture this, make the following definition

Definition 7.6.6. The field automorphism τ_q is defined by $\tau_q \colon \mathbb{C}(d, e, f, q) \to \mathbb{C}(d, e, f, q)$, where $\tau_q(q) = 1 - \frac{1}{q}$, $\tau_q(d) = e$, $\tau_q(e) = f$ and $\tau_q(f) = d$. This is the q-version of Definition 7.6.4, above.

Then we have the following corollary.

Corollary 7.6.7. *The following functional equation for* Li_6 *arises by expanding out the iterated integral* $I^-_{5,1}(\sum_i \frac{1}{a}\left[\frac{1}{1-p_i}\right] + \frac{1}{b}[p_i] + \frac{1}{c}\left[1 - \frac{1}{p_i}\right], \sum_j \frac{1}{d}\left[\frac{1}{1-q_j}\right] + \frac{1}{e}[q_j] + \frac{1}{f}\left[1 - \frac{1}{q_j}\right])$ *in two different ways.*

$$\begin{aligned}
&\sum_{q \in \{\, q_j \,\}} \mathrm{Li}_6^{\tau_p, \tau_q}\left(-\frac{1}{2a^2bc(a-d)(a-c)d}\left[\frac{t}{g(p,q)}\right] - \frac{1}{2ab^2c(a-d)(b-c)d}\left[\frac{t}{g(p,1-q)}\right]\right) + \\
&+ \sum_{p \in \{\, p_i \,\}} \mathrm{Li}_6^{\tau_p, \tau_q}\left(-\frac{1}{2cdef^2(d-f)(e-f)}\left[\frac{u}{h(q,p)}\right] + \frac{1}{2cdef^2(d-f)(e-f)}\left[\frac{u}{h(q,1-p)}\right]\right) + \\
&+ \sum_{p \in \{\, p_i \,\}} \sum_{q \in \{\, q_I \,\}} \mathrm{Li}_6^{\tau_p, \tau_q}\left(\frac{(bd-ae)(ad-be)}{12ab(a-b)de(d-e)}\left[\frac{(1-p)p}{(1-q)q}\right] + \left(\frac{b^3+2c^3}{4ab^2ce} - \frac{e^3+2f^3}{4bde^2f}\right)\left[\frac{p}{q}\right] + \right.\\
&+ \left. \left(\frac{2a^3+b^3}{4ab^2ce} + \frac{2d^3+e^3}{4bde^2f} - \frac{3}{2be}\right)[pq] - \frac{a^2+ab+b^2}{6abce}[q] \right) + \\
&+ \sum_{p \in \{\, p_i \,\}} \mathrm{Li}_6^{\tau_p}\left(-\frac{d^3-e^3}{2bdef}[p]\right) + \sum_{q \in \{\, q_j \,\}} \mathrm{Li}_6^{\tau_q}\left(\frac{a^2+ab+b^2}{ace}[q]\right) \overset{\sqcup\!\sqcup}{=} 0
\end{aligned}$$

7.6.5 Li_6 and Nielsen terms for $I^+_{5,1}$(3-term Li_3, y)

Like previously, we can also find an expression for $I^+_{5,1}$ applied to the 3-term Li_3 relation in terms of Li_6 and Nielson polylogarithms.

Recalling t from Definition 7.4.16, and r from Definition 7.4.8, we have the following.

Theorem 7.6.8. *For* $I^+_{5,1}$ *applied to the 3-term* Li_3 *functional equation, we can find explicit* Li_6 *and weight 6 Nielsen terms, and give the following identity.*

$$I^+_{5,1}\left([x] + \left[1 - \frac{1}{x}\right] + \left[\frac{1}{1-x}\right], y\right) \overset{\sqcup\!\sqcup}{=} \mathrm{Li}_6^{t,r}\left(\frac{1}{36}\left[\frac{x(1-y)^2}{(1-x)^2y}\right] - \frac{1}{9}\left[\frac{(1-x)x}{(1-y)y}\right] + \right. \tag{7.6.5a}$$

$$\left. + \left[\frac{x}{1-y}\right] - [x(1-y)] - \frac{5}{2}[(1-x)y] + \frac{1}{2}[x] + \frac{2}{3}[1-y]\right) \tag{7.6.5b}$$

$$- 4\,\mathrm{Li}_6(y) + 2S_{4,2}(y)\,. \tag{7.6.5c}$$

Remark 7.6.9. Notice, as before, that all terms except the final two in Equation 7.6.5c exhibit a visible $y \leftrightarrow \frac{1}{y}$ symmetry. The desire to use as few Nielsen polylogarithms as possible breaks the *visible* symmetry, but we do indeed have the $y \leftrightarrow \frac{1}{y}$ symmetry since

$$-4\,\mathrm{Li}_6(y) + 2S_{4,2}(y) \overset{ш}{=} -4\,\mathrm{Li}_6(\tfrac{1}{y}) + 2S_{4,2}(\tfrac{1}{y})\,.$$

So, we could replace the line from Equation 7.6.5c with

$$S_{4,2}(y) + S_{4,2}(\tfrac{1}{y})\,,$$

to give an equivalent identity, which retains the visible symmetry.

As it stands, the expression for $I^+_{5,1}$ of the 3-term Li_3 functional equation is perhaps *too* symmetric, in the sense that when $I^+_{5,1}(\text{3-term } \mathrm{Li}_3, \text{3-term } \mathrm{Li}_3)$ is converted to a functional equation for Li_6, most terms cancel. Specifically the remaining terms lead to the following.

Proposition 7.6.10. *Modulo products, the following identity holds.*

$$-2\,\mathrm{Li}_6(\tfrac{1}{1-x}) - 2\,\mathrm{Li}_6(x) - 2\,\mathrm{Li}_6(1-\tfrac{1}{x}) + S_{4,2}(x) + S_{4,2}(\tfrac{1}{1-x}) + S_{4,2}(1-\tfrac{1}{x}) \overset{ш}{=} 0\,.$$

This is still a potentially interesting result in that it gives us an expression for a certain combination of weight 6 Nielsen polylogarithms in terms of ordinary Li_6's.

7.6.6 Li_6 functional equation from $I^+_{5,1}(\text{algebraic } \mathrm{Li}_3, \text{3-term } \mathrm{Li}_3)$

Instead, if we combine this 3-term Li_3 functional equation with the algebraic Li_3 functional equation, we obtain a non-trivial Li_6 functional equation from $I^+_{5,1}(\text{algebraic } \mathrm{Li}_3, \text{3-term } \mathrm{Li}_3)$. This functional equation retains the $y \to 1-\frac{1}{y}$ symmetry, and the $p \leftrightarrow 1-p$, $a \leftrightarrow b$ antisymmetry. Since the Li_3 3-term is now in the second slot, we need to make t act on y instead of x, so make the following definition.

Definition 7.6.11. The automorphism $s\colon \mathbb{C}(y) \to \mathbb{C}(y)$ is defined by $s(y) = 1 - \frac{1}{y}$. This is like Definition 7.4.16, but t now acts on y instead of x.

In order to get a functional equation for Li_6 we need to convert the Nielsen terms to Li_6 terms. The following proposition does this.

Proposition 7.6.12. *Modulo products, the following identity holds, relating.*

$$\sum_{p \in \{\, p_i \,\}} -\frac{1}{a} S_{4,2}(1-p) + \frac{1}{b} S_{4,2}(p) \overset{ш}{=}$$
$$\sum_{p \in \{\, p_i \,\}} \frac{b-a}{a^2}\,\mathrm{Li}_6(1-p) - \frac{a-b}{b^2}\,\mathrm{Li}_6(p) - \frac{1}{a+b}\,\mathrm{Li}_6\left(1-\frac{1}{p}\right)\,.$$

Finally we can give the following Li_6 functional equation.

Corollary 7.6.13. *The following functional equation for* Li_6 *is obtained by expanding out the integral* $I^+_{5,1}$ *in two different ways, when it is applied to the algebraic* Li_3 *equation in the the first slot, and the*

3-term Li_3 *equation in the second slot.*

$$\mathrm{Li}_6^{\mu_p^-,s}\left(\frac{-1}{(a-b)(a+b)(2a+b)(a+2b)}\left[\frac{t}{g(p,y)}\right]\right)+$$
$$+\sum_{p\in\{\,p_i\,\}}\mathrm{Li}_6^{\mu_p^-,s}\left(\frac{ab}{36(a-b)}\left[\frac{(1-p)p}{(1-y)y}\right]-\frac{ab}{18(a+2b)}\left[\frac{p^2(1-y)}{(1-p)y^2}\right]+\frac{ab}{2(a+b)}\left[\frac{py}{p-1}\right]+\right.$$
$$\left.+\frac{1}{2a}\left[py\right]+\frac{1}{2a}\left[\frac{p}{y}\right]+\frac{ab}{6(a+b)}\left[\frac{p-1}{p}\right]\right)\overset{\sqcup\!\sqcup}{=}0$$

Proof. This is obtained by expanding out

$$I_{5,1}^{+}\left(\sum_i\frac{-1}{a}[1-p_i]+\frac{1}{b}[p_i],[y]+\left[1-\frac{1}{y}\right]+\left[\frac{1}{1-y}\right]\right)$$

in two different ways. We can expand out the algebraic Li_3 functional equation in the first slot using Theorem 7.6.1. Or we can expand out the 3-term Li_3 equation in the second slot using Theorem 7.6.8 and the $I_{5,1}^{+}$ version of Proposition 7.5.4. The difference of these two ways of expanding is now guaranteed to vanish modulo products.

It is possible to convert the particular combination of weight 6 Nielsen terms which appears to Li_6 terms using the identity from Proposition 7.6.12. After doing this, a common factor of

$$\frac{a^2+4ab+b^2}{a^2b^2}$$

can be cancelled from every term. This results in the desired functional equation. □

7.7 Goncharov-motivated $I_{6,1}$ identities

At this point things start to break down, although I can suggest some possible approaches which might be able to make something work. From Proposition 7.5.1, the iterated integral $I_{6,1}(x,y)$ satisfies

$$I_{6,1}(x,y)\overset{\delta}{=}-\{x\}_2\wedge\{y\}_5+\{x\}_3\wedge\{y\}_4-\{x\}_4\wedge\{y\}_3+\{x\}_5\wedge\{y\}_2\,.$$

We can consider the plus and minus symmetrisations from Definition 7.5.2, and their behaviour modulo δ. From Proposition 7.5.3 we obtain modulo δ, the symmetrisations satisfy

$$I_{6,1}^{+}(x,y)\coloneqq\frac{1}{2}(I_{6,1}(x,y)+I_{6,1}(x,\tfrac{1}{y}))\overset{\delta}{=}-\{x\}_2\wedge\{y\}_5-\{x\}_4\wedge\{y\}_3$$
$$I_{6,1}^{-}(x,y)\coloneqq\frac{1}{2}(I_{6,1}(x,y)-I_{6,1}(x,\tfrac{1}{y}))\overset{\delta}{=}\{x\}_3\wedge\{y\}_4+\{x\}_5\wedge\{y\}_2\,.$$

The following result from Proposition 7.5.4, relating $I_{6,1}^{+}(x,y)$ and $I_{6,1}^{-}(y,x)$ modulo products, means that we can restrict attention to one of the symmetrisations only. We have

$$I_{6,1}^{+}(x,y)-I_{6,1}^{-}(y,x)\overset{\sqcup\!\sqcup}{=}-3\,\mathrm{Li}_7(xy)-\frac{1}{2}\,\mathrm{Li}_7(x)-\frac{1}{2}\,\mathrm{Li}_7(y)\,.$$

Unfortunately, in neither of the symmetrisations do we find the variable x, or the variable y isolated to a single weight Bloch group term. Consequently, we can't guarantee vanishing modulo δ just by plugging in a 'simple' Li_n functional equation. All is not lost though as I can suggest two potential approaches.

7.7.1 $\mathrm{Li}_n + \mathrm{Li}_m$ functional equations

As has already been observed, the algebraic Li_4 functional equation is also a Li_2 functional equation, so might be called a $\mathrm{Li}_4 + \mathrm{Li}_2$ equation. If we substitute this into the first argument of $I^+_{6,1}(x, y)$, and look modulo δ, the factors $\{x\}_2$ and $\{x\}_4$ both vanish. We therefore expect

$$I^+_{6,1}\left(\frac{1}{a}\left[\frac{1}{1-p_i}\right] + \frac{1}{b}[p_i] + \frac{1}{c}\left[1 - \frac{1}{p_i}\right], y\right) \overset{\sqcup\!\sqcup}{=} \sum_i \alpha_i \,\mathrm{Li}_7(A_i)\,.$$

Indeed this is the case, as will be shown below.

If there also exists a (non-trivial) $\mathrm{Li}_3 + \mathrm{Li}_5$ functional equation, we could play the same game with the second argument of $I^+_{6,1}(x, y)$, to make the result vanish modulo δ. A $\mathrm{Li}_3 + \mathrm{Li}_5$ functional equation will make the factor $\{y\}_3$ and $\{y\}_5$ both vanish. Then one could expand out $I^+_{6,1}(x, y)$ in two different ways to obtain a functional equation for Li_7 – indeed a family of functional equations, because the $\mathrm{Li}_2 + \mathrm{Li}_4$ algebraic equation is itself a family of functional equations.

I am hopeful that such a (non-trivial) $\mathrm{Li}_3 + \mathrm{Li}_5$ functional equation exists, although it is probably rather complicated. Certainly $[y] - [\frac{1}{y}]$ is an example of a $\mathrm{Li}_3 + \mathrm{Li}_5$ functional equation. Unfortunately it is not useful for our purposes. It makes $I^+_{6,1}(x, y)$ vanish identically because we have already symmetrised over $[y] + [\frac{1}{y}]$. Nevertheless, it shows that such functional equations may *in principal* exist.

7.7.2 Further symmetrisation

Another approach is to further symmetrise the integral $I^-_{6,1}$, in an effort to isolate the variables. For example, we can make the $\{y\}_2$ term vanish using the Li_2 functional equation $[y] + [1 - y]$. Since $[y] + [1 - y]$ is not Li_4 functional equation, the term $\{y\}_4$ does not vanish. Indeed could make the following definition.

Definition 7.7.1 (2-term symmetrisation $\widehat{I^-_{6,1}}$)**.** The *2-term* symmetrisation of $I^-_{6,1}(x, y)$ is defined to be

$$\widehat{I^-_{6,1}}(x, y) \coloneqq I^-_{6,1}(x, y) + I^-_{6,1}(x, 1 - y)\,.$$

From this we obtain the following proposition

Proposition 7.7.2. *Modulo δ, the 2-term symmetrisation satisfies*

$$\widehat{I^-_{6,1}}(x, y) = I^-_{6,1}(x, [y] + [1 - y]) \overset{\delta}{=} \{x\}_3 \wedge \{y\}_4 + \{x\}_3 \wedge \{1 - y\}_4 \;.$$

So we see that modulo δ, the x argument of $\widehat{I^-_{6,1}}(x, y)$ only occurs in the weight 3 Bloch group. By substituting any Li_3 functional equation for x, we can guarantee the result vanishes modulo δ. We therefore expect the result to be expressible in terms of Li_7's. Indeed this is the case for the algebraic Li_3 functional equation, as given below.

If there now also exists a functional equation for $\mathrm{Li}_4(y) + \mathrm{Li}_4(1-y)$, we can substitute this in for the y argument, to make the result vanish modulo δ. To clarify, I would like to find arguments A_i, and coefficients α_i such that

$$\sum_i \alpha_i \left(\mathrm{Li}_4(A_i) + \mathrm{Li}_4(1-A_i)\right) \overset{\sqcup\!\sqcup}{=} 0\,.$$

Given this, we then can play the same game as always: by expanding out $\widehat{I^-_{6,1}}(x,y)$ in two different ways we would again obtain a family of functional equations for Li_7. I am hopeful that such a $\mathrm{Li}_4(y) + \mathrm{Li}_4(1-y)$ functional equations exists, although I cannot give even a trivial example.

7.7.3 Results

7.7.3.1 Li_7 terms for $I^+_{6,1}$(algebraic Li_4, y)

Recalling τ from Definition 7.6.4, and r from Definition 7.4.8, we have the following.

Theorem 7.7.3. *Then for $I^+_{6,1}$ applied to the Li_4 algebraic equation we can find explicit Li_7 terms, and give the following identity.*

$$I^+_{6,1}\left(\frac{1}{a}\left[\frac{1}{1-p_i}\right] + \frac{1}{b}[p_i] + \frac{1}{d}\left[1-\frac{1}{p_i}\right], y\right) \overset{\sqcup\!\sqcup}{=} \tag{7.7.1}$$

$$\mathrm{Li}_7^{\tau,r^-}\left(\frac{1}{ab^2c(b-a)(a+2b)(2a+b)}\left[\frac{t}{g(p,y)}\right]\right) + \frac{c^2-ab}{ac}\mathrm{Li}_7(y) + \tag{7.7.2}$$

$$+\sum_{p\in\{\,p_i\,\}} \mathrm{Li}_7^{\tau,r^-}\left(\frac{1}{18(b-a)}\left[\frac{(1-y)y}{(1-p)p}\right] - \frac{1}{72(2a+b)}\left[\frac{(1-p)^2y}{p(1-y)^2}\right] + \right. \tag{7.7.3}$$

$$\left. -\frac{2a+7b}{4b^2}[py] - \frac{1}{2b}\left[\frac{p}{1-y}\right] + \frac{1}{2b}[p(1-y)] - \frac{1}{4b}[p]\right) \tag{7.7.4}$$

Data. Mathematica verification for (a,b) equal to $(1,2)$, $(1,3)$, $(1,4)$, $(2,1)$ and $(2,3)$ □

7.7.3.2 Li_7 terms for $\widehat{I^-_{6,1}}$(algebraic Li_3, y)

Notice that $\widehat{I^-_{6,1}}(x,y)$ is only symmetric under $y \mapsto 1-y$, and not under $y \mapsto \frac{1}{y}$. This means we need to change how $\mathrm{Li}_7^{\sigma,r}$ is symmetrised, and so using a different automorphism. Make the following definition

Definition 7.7.4. The automorphism $m\colon \mathbb{C}(y) \to \mathbb{C}(y)$ is defined by $m(y) = 1-y$. In this definition, m is a mnemonic for "one *minus* y".

Recall also μ from Definition 7.4.10.

Theorem 7.7.5. *For $\widehat{I^-_{6,1}}$ applied to the Li_3 algebraic equation we can find explicit Li_6 terms, and give the following identity.*

$$\widehat{I^-_{6,1}}\left(\sum_i -\frac{1}{a}[1-p_i] + \frac{1}{b}[p_i], y\right) \overset{\sqcup\!\sqcup}{=} \tag{7.7.5}$$

$$\mathrm{Li}_7^{\mu^-,m}\left(\frac{-1}{2(ab)^2(b-a)(a+2b)(2a+b)}\left[\frac{t}{g(p,y)}\right]-\frac{1}{a^2bc(b-a)(a+2b)(2a+b)}\left[\frac{t}{g(\frac{1}{1-p},y)}\right]\right)+ \tag{7.7.6}$$

$$+\sum_{p_i\in\{\,p\,\}}\mathrm{Li}_7^{\mu^-,m}\left(\frac{2a+7b}{4b^2}[py]-\frac{2a+9b}{4b^2}\left[\frac{p}{y}\right]-\frac{1}{2a}\left[\frac{1-p}{1-1/y}\right]+\frac{1}{2c}\left[\frac{1-1/p}{y}\right]+\right. \tag{7.7.7}$$

$$-\frac{1}{36(2a+b)}\left[-\frac{(1-p)^2(1-y)y}{p}\right]+\frac{1}{36(b-a)}\left[\frac{(1-p)p}{(1-y)y}\right]+ \tag{7.7.8}$$

$$\left.+\frac{1}{36(2a+b)}\left[\frac{(1-p)^2(1-y)}{py^2}\right]-\frac{1}{36(b-a)}\left[-\frac{(1-p)p(1-y)^2}{y}\right]\right) \tag{7.7.9}$$

Data. Mathematica verification for (a,b) equal to $(1,2)$, $(1,3)$, $(1,4)$, $(2,1)$ and $(2,3)$ □

7.7.3.3 Li_7 and Nielsen terms for $\widehat{I_{6,1}^-}$(3-term Li_3, y)

We can also give an expression for the 3-term Li_3 functional equation.

Recall t from Definition 7.4.16 and m from Definition 7.7.4. We have the following.

Theorem 7.7.6. *For $\widehat{I_{6,1}^-}(x,y)$ applied to the 3-term Li_3 equation, we can find explicit Li_7 and weight 7 Nielsen terms, and give the following identity.*

$$\widehat{I_{6,1}^-}\left([x]+\left[\frac{1}{1-x}\right]+\left[1-\frac{1}{x}\right],y\right)\overset{\sqcup\!\sqcup}{=}\mathrm{Li}_7^{t,m}\left(-\frac{1}{36}\left[\frac{x^2(1-y)}{y^2(1-x)}\right]+\frac{1}{36}\left[\frac{(1-x)x}{(1-y)y}\right]+\right.$$
$$\left.+\frac{1}{2}\left[\frac{x(1-y)}{y(1-x)}\right]+\frac{5}{4}[xy]-\frac{7}{4}\left[\frac{x}{y}\right]-\frac{2}{3}[y]-\frac{1}{6}\left[-\frac{1-y}{y}\right]\right)+$$
$$+S_{5,2}(y)+S_{5,2}(1-y)\,.$$

7.8 Further work

7.8.1 Approach for $I_{7,1}$ and beyond

From Proposition 7.5.1, the integral $I_{7,1}(x,y)$ satisfies

$$I_{7,1}(x,y)\overset{\delta}{=}-\{x\}_2\wedge\{y\}_6+\{x\}_3\wedge\{y\}_5-\{x\}_4\wedge\{y\}_4+\{x\}_5\wedge\{y\}_3-\{x\}_6\wedge\{y\}_2\,.$$

Using Proposition 7.5.3, we find that the symmetrisations from Definition 7.5.2 satisfy the following, modulo δ.

$$I_{7,1}^+(x,y)\coloneqq\tfrac{1}{2}(I_{7,1}(x,y)+I_{7,1}(x,\tfrac{1}{y}))\overset{\delta}{=}\{x\}_3\wedge\{y\}_5+\{x\}_5\wedge\{y\}_3$$
$$I_{7,1}^-(x,y)\coloneqq\tfrac{1}{2}(I_{7,1}(x,y)-I_{7,1}(x,\tfrac{1}{y}))\overset{\delta}{=}-\{x\}_2\wedge\{y\}_6-\{x\}_4\wedge\{y\}_4-\{x\}_6\wedge\{y\}_2\,.$$

7.8.1.1 Symmetrising with $\{x\}_2 + \{1-x\}_2$

Symmetristing $I^-_{7,1}(x,y)$ to

$$\widehat{I^-_{7,1}}(x,y) \coloneqq I^+_{7,1}([x]+[1-x],[y]+[1-y])$$

gives

$$\widehat{I^-_{7,1}}(x,y) \overset{\delta}{=} -(\{x\}_4 + \{1-x\}_4) \wedge (\{y\}_4 + \{1-y\}_4)\,.$$

If we can find a functional equation for $\mathrm{Li}_4(x) + \mathrm{Li}_4(1-x)$, we can substitute it as the x argument, or as the y argument to $\widehat{I^-_{7,1}}$, and get a result which is 0 modulo δ. This means the result should be expressible in terms of Li_8. So with a functional equation for $\mathrm{Li}_4(x) + \mathrm{Li}_4(1-x)$, we would also be able apply it here to find a functional equation for Li_8.

7.8.1.2 Using $\mathrm{Li}_3 + \mathrm{Li}_5$ functional equations

Similarly, a functional equation for $\mathrm{Li}_3 + \mathrm{Li}_5$, substituted into the x or y argument of $I^-_{7,1}(x,y)$ makes the result vanish modulo δ. The result of this should be expressible in terms of Li_8, we could then use to find a functional equation for Li_8. Whichever approach above succeeds in finding a family of Li_7 functional equations, could be immediately applied to find at least one Li_8 functional equation.

7.8.1.3 Symmetrising with Li_3 equations

Alternatively, and maybe more ambitiously, we can symmetrise $I^+_{7,1}(x,y)$ to, say,

$$\widetilde{I^+_{7,1}}(x,y) \coloneqq I^+_{7,1}\left([x] + \left[\frac{1}{1-x}\right] + \left[1-\frac{1}{x}\right], y\right)\,.$$

This kills the $\{x\}_3$ factor, leaving

$$\widetilde{I^+_{7,1}}(x,y) \overset{\delta}{=} \left(\{x\}_5 + \left\{\frac{1}{1-x}\right\}_5 + \left\{1-\frac{1}{x}\right\}_5\right) \wedge \{y\}_3\,.$$

Substituting in a Li_3 functional equation for y makes the result vanish modulo δ, giving us a Li_8 combination. And a functional equation for $\mathrm{Li}_5(x) + \mathrm{Li}_5\left(\frac{1}{1-x}\right) + \mathrm{Li}_5\left(1-\frac{1}{x}\right)$, could lead to a family of functional equations for Li_8.

We can give an expression when the 3-term Li_3 functional equation is used. Recall t from Definition 7.4.16. We also need the y-version s from Definition 7.6.11. Then we have the following.

Theorem 7.8.1. *For $\widetilde{I^+_{7,1}}(x,y)$ applied to the 3-term Li_3 equation, we can find explicit Li_8 and weight 8 Nielsen terms, and give the following identity.*

$$\widetilde{I^+_{7,1}}\left(x, [y] + \left[\frac{1}{1-y}\right] + \left[1-\frac{1}{y}\right]\right) \overset{ш}{=} \mathrm{Li}_8^{t,s}\left(-\frac{1}{36}\left[\frac{(1-x)x}{(1-y)y}\right] + \frac{7}{4}\left[\frac{x}{y}\right] + \frac{7}{4}[xy] - \frac{3}{2}[x] - [y]\right) +$$
$$+ S_{6,2}\left([x] + \left[\tfrac{1}{1-x}\right] + \left[1-\tfrac{1}{x}\right]\right) + S_{6,2}\left([y] + \left[\tfrac{1}{1-y}\right] + \left[1-\tfrac{1}{y}\right]\right)$$

Presumably, an expression for $\widetilde{I^{+}_{7,1}}(x, y)$ applied to the algebraic Li_3 equation can also be found, with a similar form to Theorem 7.7.5. Since $\widetilde{I^{+}_{7,1}}(x, y)$ is defined using a symmetrisation coming from the 3-term Li_3 equation, we anticipate weight 8 Nielsen terms appearing. A different symmetrisation of $I^{+}_{7,1}$, say using the rationally parameterisable $a = 1, b = 2$ case (see Remark 7.3.2) of the algebraic Li_3, could eliminate some of the Nielsen terms.

7.8.1.4 Using $\mathrm{Li}_2 + \mathrm{Li}_4$ functional equations

Another potential approach comes from noticing that substituting the $\mathrm{Li}_2 + \mathrm{Li}_4$ functional equation in the x argument leaves only $\{y\}_2$. So the result vanishes modulo δ for any Li_2 functional equation. The same thing holds swapping x and y. One has

$$I^{m}_{7,1}\left(\sum_i \frac{1}{a}\left[\frac{1}{1-p_i}\right] + \frac{1}{b}[p_i] + \frac{1}{d}\left[1 - \frac{1}{p_i}\right], \sum_j \frac{1}{a'}\left[\frac{1}{1-q_j}\right] + \frac{1}{b'}[q_j] + \frac{1}{c'}\left[1 - \frac{1}{q_j}\right]\right) \overset{\delta}{=} 0\,.$$

But one can expand this out in two ways. Either in the second slot:

$$\begin{aligned}
0 \overset{\delta}{=} I^{-}_{7,1}&\left(\sum_i \tfrac{1}{a}\left[\tfrac{1}{1-p_i}\right] + \tfrac{1}{b}[p_i] + \tfrac{1}{d}\left[1 - \tfrac{1}{p_i}\right], \sum_j \tfrac{1}{a'}\left[\tfrac{1}{1-q_j}\right] + \tfrac{1}{b'}[q_j] + \tfrac{1}{c'}\left[1 - \tfrac{1}{q_j}\right]\right) \\
= I^{-}_{7,1}&\left(\sum_i \tfrac{1}{a}\left[\tfrac{1}{1-p_i}\right] + \tfrac{1}{b}[p_i] + \tfrac{1}{d}\left[1 - \tfrac{1}{p_i}\right], \sum_j \tfrac{1}{a'}\left[\tfrac{1}{1-q_j}\right]\right) + \\
&+ I^{-}_{7,1}\left(\sum_i \tfrac{1}{a}\left[\tfrac{1}{1-p_i}\right] + \tfrac{1}{b}[p_i] + \tfrac{1}{d}\left[1 - \tfrac{1}{p_i}\right], \sum_j \tfrac{1}{b'}[q_j]\right) + \\
&+ I^{-}_{7,1}\left(\sum_i \tfrac{1}{a}\left[\tfrac{1}{1-p_i}\right] + \tfrac{1}{b}[p_i] + \tfrac{1}{d}\left[1 - \tfrac{1}{p_i}\right], \sum_j \tfrac{1}{c'}\left[1 - \tfrac{1}{q_j}\right]\right)\,,
\end{aligned}$$

where each $I^{-}_{7,1}$ vanishes modulo δ, so is morally a sum of Li_8's. Or similarly in the first slot,

$$\begin{aligned}
= I^{-}_{7,1}&\left(\sum_i \tfrac{1}{a}\left[\tfrac{1}{1-p_i}\right], \sum_j \tfrac{1}{a'}\left[\tfrac{1}{1-q_j}\right] + \tfrac{1}{b'}[q_j] + \tfrac{1}{c'}\left[1 - \tfrac{1}{q_j}\right]\right) + \\
&+ I^{-}_{7,1}\left(\sum_i \tfrac{1}{b}[p_i], \sum_j \tfrac{1}{a'}\left[\tfrac{1}{1-q_j}\right] + \tfrac{1}{b'}[q_j] + \tfrac{1}{c'}\left[1 - \tfrac{1}{q_j}\right]\right) + \\
&+ I^{-}_{7,1}\left(\sum_i \tfrac{1}{d}\left[1 - \tfrac{1}{p_i}\right], \sum_j \tfrac{1}{a'}\left[\tfrac{1}{1-q_j}\right] + \tfrac{1}{b'}[q_j] + \tfrac{1}{c'}\left[1 - \tfrac{1}{q_j}\right]\right)\,,
\end{aligned}$$

where each $I^{-}_{7,1}$ vanishes modulo δ, and so is morally the sum of other Li_8's. With luck, the combinations obtained when expanding out the second slot will differ from the combinations obtained when expanding out the first slot. So the difference will vanish modulo products, and could give a Li_8 functional equation.

Unfortunately it is not clear that the two combinations should necessarily be *different*. This expansion does not involve some independent variable y which has arguments substituted in later, so we could just end up with two different ways of grouping the same Li_8 terms. And the difference would trivially cancel to 0. Thus far, the computation to attempt this has been difficult to finish due to excessive memory requirements.

7.8.2 Approach for depth 2 identities

It would also be desirable to find some generalisation of these ideas to higher depth iterated integrals. Goncharov's approach uses 'simple' low weight Li_n functional equations substituted into depth 2 iterated integrals to derive more complicated higher weight Li_n functional equations.

One possible generalisation to consider could come from using Li_n functional equations substituted into (carefully chosen!) depth 3 iterated integrals, in order to try to derive more 'interesting' identities for depth 2 integrals. Currently, I have no specific results in this direction, but I can at least illustrate the way.

The depth 3 iterated integral $I_{4,1,1}(x,y,z)$ seems to satisfy the following, 'modulo δ^2'

$$I_{4,1,1}(x,y,z) \overset{\delta^2}{=} \{x\}_2 \wedge \left(\left\{ \frac{z}{y} \right\}_2 \wedge \{z\}_2 \right) + \left\{ \frac{z}{y} \right\}_2 \wedge (\{x\}_2 \wedge \{z\}_2) \,.$$

Therefore, the following 'symmetrised' version of $I_{4,1,1}$

$$\widetilde{I_{4,1,1}}(x,y,z) \coloneqq I_{4,1,1}(x, z/y, z)$$

satisfies

$$\widetilde{I_{4,1,1}}(x,y,z) \overset{\delta^2}{=} \{x\}_2 \wedge (\{y\}_2 \wedge \{z\}_2) + (\{x\}_2 \wedge \{z\}_2) \wedge \{y\}_2 \,.$$

Remark 7.8.2. There is of course a question surrounding what 'modulo δ^2' means, and how it should be interpreted. In the Lie coalgebra $\mathcal{L}_\bullet$, we have $\delta^2 = 0$ identically, since δ is a Lie cobracket. In the weight 6 case we have the exact sequence

$$0 \to \mathcal{B}_6 \to \mathcal{L}_6 \to \mathcal{B}_3 \wedge \mathcal{B}_3 \oplus \mathcal{B}_2 \otimes \mathcal{L}_4 \to \bigwedge^3 \mathcal{B}_2 \to 0 \,,$$

so that δ^2 is a map $\delta^2 \colon \mathcal{L}_6 \to \bigwedge^3 \mathcal{B}_2$, whereas in the above result, we land in $(\bigwedge^2 \mathcal{B}_2) \wedge \mathcal{B}_2 \oplus \mathcal{B}_2 \wedge (\bigwedge^2 \mathcal{B}_2)$. We then need to make the natural identification $\bigwedge^3 \mathcal{B}_2 \cong (\bigwedge^2 \mathcal{B}_2) \wedge \mathcal{B}_2 \oplus \mathcal{B}_2 \wedge (\bigwedge^2 \mathcal{B}_2)$, after which the two terms $\{x\}_2 \wedge (\{y\}_2 \wedge \{z\}_2) + (\{x\}_2 \wedge \{z\}_2) \wedge \{y\}_2$ can be made to cancel.

Therefore perhaps the correct thing to do is to consider just one of these components as a time. A result already vanishing in each separate $\mathcal{B}_2 \wedge (\mathcal{B}_2 \wedge \mathcal{B}_2)$ and $(\mathcal{B}_2 \wedge \mathcal{B}_2) \wedge \mathcal{B}_2$ component should give some further information about the structure of the original iterated integral. Moreover, since each depth 2 iterated integral $I_{a,b}(x,y)$ has the form $\sum_i \{\alpha_i\}_{n_i} \wedge \{\beta_i\}_{m_i}$ modulo δ, each component of the result $I_{a,b}(x,y)$ 'modulo δ^2' vanishes already. Therefore the 'modulo δ^2' process should detect when something is a depth 2 iterated integral.

From the above expression for $\widetilde{I_{4,1,1}}(x,y,z)$ 'modulo δ^2', we see that plugging in a Li_2 functional equation to any of the arguments x, or y, or z forces the result to vanish 'modulo δ^2'. One then could expect the result to be expressible in terms of depth 2 iterated integrals only modulo δ. If we can find an expression for this when a Li_2 equation $L_2 = \sum_i a_i [A_i] \in \ker \delta_2$ is plugged into the x slot, and an expression when a(nother) Li_2 equation $L_2' = \sum_i b_i [B_i] \in \ker \delta_2$ is plugged into the y slot, we can expand

$$\widetilde{I_{4,1,1}}(L_2, L_2', z)$$

in two different ways as a sum of depth 2 iterated integrals. The difference then necessarily vanishes modulo δ giving a functional equation for depth 2 iterated integrals. Then one could even attempt to find the Li_n terms to get a identity which holds modulo products.

Bibliography

[Abe81] Niels Henrik Abel. “Oeuvres Completes, vol. 2”. In: *Christiana, Christiana, Ten, USA* (1881).

[Apé79] R. Apéry. “Irrationalité de $\zeta(2)$ et $\zeta(3)$”. In: *Astérisque* 61 (1979), pp. 11–13.

[BB02] Douglas Bowman and David M. Bradley. “The Algebra and Combinatorics of Shuffles and Multiple Zeta Values”. In: *Journal of Combinatorial Theory, Series A* 97.1 (2002), pp. 43–61. arXiv: `math/0310082 [math.CO]`.

[BB06] Jonathan M. Borwein and David M. Bradley. “Thirty-two Goldbach variations”. In: *International Journal of Number Theory* 2.01 (2006), pp. 65–103. arXiv: `math/0502034 [math.NT]`.

[BBB97] J. M. Borwein, D. M. Bradley, and D. J. Broadhurst. “Evaluations of k-fold Euler/Zagier sums: a compendium of results for arbitrary k”. In: *The Electronic Journal of Combinatorics* 4.2 (1997), #R5. arXiv: `hep-th/9611004`.

[BBBL01] Jonathan Borwein, David Bradley, David Broadhurst, and Petr Lisoněk. “Special values of multiple polylogarithms”. In: *Transactions of the American Mathematical Society* 353.3 (2001), pp. 907–941. arXiv: `math/9910045 [math.CA]`.

[BBBL98] Jonathan M. Borwein, David M. Bradley, David J. Broadhurst, and Petr Lisoněk. “Combinatorial aspects of multiple zeta values”. In: *The Electronic Journal of Combinatorics* 5 (1998), #R38. arXiv: `math/9812020 [math.NT]`.

[Blo00] Spencer Bloch. *Higher regulators, algebraic K-theory, and zeta functions of elliptic curves.* Vol. 11. American Mathematical Soc., 2000.

[Blo77] Spencer Bloch. “Applications of the dilogarithm function in algebraic K-theory and algebraic geometry”. In: *Proceedings of the International Symposium on Algebraic Geometry, Kyoto.* 1977, pp. 103–115.

[Bro] Francis Brown. “Representation theory of polylogarithms”. (Unpublished).

[Bro09] Francis Brown. “Multiple zeta values and periods of moduli spaces $\mathfrak{M}_{0,n}$”. In: *Annales scientifiques de l’Ecole normale supérieure.* Vol. 42.3. Elsevier. 2009, pp. 371–489. arXiv: `math/0606419 [math.AG]`.

[Bro12a] Francis Brown. “Mixed Tate Motives over $\mathbb{Z}$”. In: *Annals of Mathematics* 175.2 (2012), pp. 949–976. arXiv: 1102.1312 [math.AG].

[Bro12b] Francis C. S. Brown. “On the decomposition of motivic multiple zeta values”. In: *Galois-Teichmüller Theory and Arithmetic Geometry.* Vol. 63. Advanced Studies in Pure Mathematics. The Mathematical Society of Japan, 2012, pp. 31–58. arXiv: 1102.1310 [math.NT].

[BW11] Christian Bogner and Stefan Weinzierl. “Feynman graphs in perturbative quantum field theory”. In: *Asymptotics in Dynamics, Geometry and PDEs; Generalized Borel Summation.* Vol. II. Springer, 2011, pp. 1–26. arXiv: 0912.4364 [math-ph].

[BZ] Jonathan M. Borwein and Wadim Zudilin. *Multiple Zeta Values Lecture Notes.* URL: https://carma.newcastle.edu.au/MZVs/mzv.pdf.

[Cha15] Steven Charlton. “$\zeta(\{\{2\}^m, 1, \{2\}^m, 3\}^n, \{2\}^m)/\pi^{4n+2m(2n+1)}$ is rational”. In: *Journal of Number Theory* 148 (2015), pp. 463–477. arXiv: 1306.6775 [math.NT].

[Che77] Kuo-Tsai Chen. “Iterated Path Integrals”. In: *Bulletin of the American Mathematical Society* 83.5 (1977), pp. 831–879.

[Dan08] Nicusor Dan. *Sur la conjecture de Zagier pour $n = 4$.* 2008. arXiv: 0809.3984 [math.KT].

[Dan11] Nicusor Dan. *Sur la conjecture de Zagier pour $n = 4$. II.* 2011. arXiv: 1101.1557 [math.KT].

[DDDS10] Vittorio Del Duca, Claude Duhr, and Vladimir A. Smirnov. “The two-loop hexagon Wilson loop in $\mathcal{N} = 4$ SYM”. In: *Journal of High Energy Physics* 2010.5 (2010), pp. 1–120. arXiv: 1003.1702 [hep-th].

[DGR12] Claude Duhr, Herbert Gangl, and John R. Rhodes. “From polygons and symbols to polylogarithmic functions”. In: *Journal of High Energy Physics* 2012.10 (2012), pp. 1–79. arXiv: 1110.0458 [math-ph].

[Eul43] Leonhard Euler. “De summis serierum reciprocarum ex potestatibus numerorum naturalium ortarum dissertatio altera in qua eaedem summationes ex fonte maxime diverso derivantur”. In: *Miscellanea Berolinensia* 7.1743 (1743), pp. 172–192.

[Eul75] L. Euler. “Meditationes circa singulare serierum genus”. In: *Opera Omnia I-15* (1775), pp. 217–267.

[FTW16] Hjalte Frellesvig, Damiano Tommasini, and Christopher Wever. “On the reduction of generalized polylogarithms to Li_n and $\mathrm{Li}_{2,2}$ and on the evaluation thereof”. In: *Journal of High Energy Physics* 3.2016 (2016), pp. 1–36. arXiv: 1601.02649 [hep-ph].

[Fur03] Hidekazu Furusho. “The multiple zeta value algebra and the stable derivation algebra”. In: *Publications of the Research Institute for Mathematical Sciences* 39 (2003), pp. 965–720. arXiv: math/0011261 [math.NT].

[Gan00] Herbert Gangl. “Some computations in weight 4 motivic complexes”. In: *Regulators in analysis, geometry and number theory*. Springer, 2000, pp. 117–125. URL: http://www.maths.dur.ac.uk/~dma0hg/motcoh.pdf.

[Gan03] Herbert Gangl. “Functional equations of higher logarithms”. In: *Selecta Mathemaica* 9 (2003), pp. 361–379.

[Gan16] Herbert Gangl. *Multiple polylogarithms in weight 4*. 2016. arXiv: 1609.05557 [math.NT].

[Gan95] Herbert Gangl. “Funktionalgleichungen von Polylogarithmen”. PhD thesis. Mathematisches Institut der Universität Bonn, 1995.

[GGL09] H. Gangl, A. B. Goncharov, and A. Levin. “Multiple polylogarithms, polygons, trees and algebraic cycles”. In: *Algebraic Geometry, Seattle 2005*. Vol. 80.2. Proceedings of Symposia in Pure Mathematics. American Mathematical Society, 2009, pp. 547–593. arXiv: math/0508066 [math.NT].

[GKZ06] H. Gangl, M. Kaneko, and D. Zagier. “Double Zeta Values and Modular Forms”. In: *Automorphic Forms and Zeta Functions*. World Scientific, 2006, pp. 71–106.

[Gla16] Claire Glanois. “Periods of the motivic fundamental groupoid of $\mathbb{P}^1 \setminus \{ 0, \mu_N, \infty \}$”. PhD thesis. Université Pierre et Marie Curie, 2016.

[Gon01] Alexander B. Goncharov. “Multiple polylogarithms and mixed Tate motives”. In: (2001). arXiv: math/0103059 [math.AG].

[Gon02] A. B. Goncharov. *Periods and mixed motives*. 2002. arXiv: math/0202154 [math.AG].

[Gon05] A. B. Goncharov. “Galois symmetries of fundamental groupoids and noncommutative geometry”. In: *Duke Mathematical Journal* 128.2 (2005), pp. 209–284. arXiv: math/0208144 [math.AG].

[Gon91] A. B. Goncharov. “The Classical Trilogarithm, Algebraic K-Theory of Fields and Dedekind Zeta Funtions”. In: *Bulletin (New Series) of the American Mathematical Society* 24.1 (1991), pp. 155–162.

[Gon94] Alexander B. Goncharov. *Polylogarithms and motivic Galois groups*. Motives (Seattle, WA, 1991), 1994.

[Gon95a] Alexander B. Goncharov. “Geometry of configurations, polylogarithms, and motivic cohomology”. In: *Advances in Mathematics* 114.2 (1995), pp. 197–318.

[Gon95b] Alexander B. Goncharov. “Polylogarithms in Arithmetic and Geometry”. In: *Proceeings of the Internationanl Congress of Mathematics*. Vol. 1 (Zürich 1994). Birkhäuser Basel, 1995, pp. 374–387.

[Gon98] Alexander B. Goncharov. “Multiple polylogarithms, cyclotomy and modular complexes”. In: *Mathematical Research Letters* 5 (1998), pp. 497–516.

[GSVV10] Alexander B. Goncharov, Marcus Spradlin, C. Vergu, and Anastasia Volovich. “Classical polylogarithms for amplitudes and Wilson loops”. In: *Physical review letters* 105.15 (2010), p. 151605. arXiv: `1006.5703 [hep-th]`.

[HO03] Michael E. Hoffman and Yasuo Ohno. “Relations of multiple zeta values and their algebraic expression”. In: *Journal of Algebra* 262.2 (2003), pp. 332–347. arXiv: `math/0010140 [math.QA]`.

[Hof05] Michael E. Hoffman. “Algebraic Aspects of Multiple Zeta Values”. In: *Zeta Functions, Topology and Quantum Physics*. Springer US, 2005, pp. 51–73. arXiv: `math/0309425 [math.QA]`.

[Hof92] Michael E. Hoffman. “Multiple Harmonic Series”. In: *Pacific Journal of Mathematics* 152.2 (1992), pp. 275–290.

[Hof97] Michael E. Hoffman. “The Algebra of Multiple Harmonic Series”. In: *Journal of Algebra* 194 (1997), pp. 477–495.

[IKZ06] Kentaro Ihara, Masanobu Kaneko, and Don Zagier. “Derivation and double shuffle relations for multiple zeta values”. In: *Compositio Mathematica* 142.02 (2006), pp. 307–338.

[Kum40] E. E. Kummer. “Uber die Transcendeten, welche aus wiederholten Integrationen rationaler Formeln entstehen”. In: *Journal für die reine und angewandte Mathematik (Crelle)* 21 (1840), pp. 74–90.

[LD28] IA Lappo-Danilevsky. “Resolution algorithmique des problem es reguliers de Poincare et de Riemann”. In: *Journal de la Société Physico-Mathématique de Léningrade* 2 (1928), p. 94.

[Lei55] G. W. Leibniz. *Mathematische Schriften*. Ed. by C. I. Gerhardt. Vol. 3. A. Asher, 1855, pp. 336–338.

[Mun09] Shuichi Muneta. “A note on evaluations of multiple zeta values”. In: *Proceedings of the American Mathematical Society* 137.3 (2009), pp. 931–935. arXiv: `0802.4331 [math.NT]`.

[Nie09] Niels Nielsen. “Der Eulersche Dilogarithmus und seine Verallgemeinerungen”. In: *Nova Acta Leopoldina* 90 (1909), p. 123.

[Pan15] Erik Panzer. *The parity theorem for multiple polylogarithms*. 2015. arXiv: `1512.04482 [math.NT]`.

[Rho12] John Richard Rhodes. “On the kernel of the symbol map for multiple polylogarithms”. PhD thesis. Durham University, 2012. URL: `http://etheses.dur.ac.uk/3905/`.

[Riv00] T. Rivoal. “La function zêta de Riemann prend une infinité de valeurs irrationalles aux entiers impairs”. In: *Comptes Rendus de l’Académie des Sciences - Series I - Mathematics* 331.4 (2000), pp. 267–270.

[RV00] Ettore Remiddi and Jos A. M. Vermaseren. “Harmonic polylogarithms”. In: *International Journal of Modern Physics A* 15.05 (2000), pp. 725–754. arXiv: `hep-ph/9905237 [hep-ph]`.

[Sch46] W. Schaeffer. In: *Journal für die reine und angewandte Mathematik (Crelle)* 30 (1846), pp. 277–295.

[Sou15] Ismaël Souderes. *Équations fonctionnelles du dilogarithme*. 2015. arXiv: `1509.02869 [math.AG]`.

[Ste52] Robert Steinberg. "Solution of Advanced Problem 4431". In: *American Mathematical Monthly* 59 (1952), pp. 471–472.

[Sus86] A. A. Suslin. "Algebraic K-Theory of Fields". In: *International Congress of Mathematicians*. 1986, pp. 222–244.

[Ter02] Tomohide Terasoma. "Mixed Tate motives and multiple zeta values". In: *Inventiones mathematicae* 149 (2002), pp. 339–369. arXiv: `math/0104231 [math.AG]`.

[Tsu04] Hirofumi Tsumura. "Combinatorial relations for Euler-Zagier sums". In: *Acta Arithmetica* 111 (2004), pp. 27–42.

[Ver] Cristian Vergu. *Polylogarithms and Physical Applications*. URL: `http://www.maths.dur.ac.uk/events/Meetings/LMS/2013/PNTPP13/talks/0190vergu.pdf`.

[Wei07] Stefan Weinzierl. *Feynman integrals and multiple polylogarithms*. 2007. arXiv: `0705.0900 [hep-ph]`.

[Woj96] Zdzisław Wojtkowiak. "Functional equations of iterated integrals with regular singularities". In: *Nagoya Mathematical Journal* 142 (1996), pp. 145–159.

[Zag12] Don Zagier. "Evaluation of the multiple zeta values $\zeta(2,\dots,2,3,2,\dots,2)$". In: *Annals of Mathematics* 175.2 (2012), pp. 977–1000.

[Zag86] D. Zagier. "Hyperbolic manifolds and special values of Dedekind zeta functions". In: *Inventiones Mathematicae* 83 (1986), pp. 285–301.

[Zag91] D. Zagier. "Polylogarithms, Dedekind zeta functions and the algebraic K-theory of fields". In: *Arithmetic Algebraic Geometry*. Ed. by G. van der Geer, F. Oort, and J. Steenbrink. Vol. 89. Progress in mathematics. Birkhäuser Boston, 1991, pp. 391–430.

[Zag94] D. Zagier. "Values of Zeta Functions and their applications". In: *Proceedings of the ECM Paris 1992*. Vol. 120. Progress in Mathematics. 1994, pp. 497–512.

[Zha08] Jianqiang Zhao. "An exotic shuffle relation for multiple zeta values". In: *Archiv der Mathematik* 91.5 (2008), pp. 409–415. arXiv: `0707.3244 [math.NT]`.

[Zha16] Jianqiang Zhao. *Multiple zeta functions, mltiple polylogarithms and their special values*. Series on number theory and its applications. World Scientific Publishing Company, 2016. ISBN: 9789814689410.

[Zud03] V. V. Zudilin. "Algebraic relations for multiple zeta values". In: *Russian Mathematical Surveys* 58.1 (2003), pp. 3–32.

Software

[GP] The PARI group. *GP/Pari Calculator*. URL: http://pari.math.u-bordeaux.fr/.

[MA] Wolfram Research. *Mathematica*. Version 8.0.1.0 – 10.0.2.0.

[MESA] Danylo Radchenko. *MESA. A SageMath module for finding functional equations for polylogarithms.* Private release currently. Public release is planned after further development and testing.

[PT] Claude Duhr. *PolylogTools package for Mathematica.*

[TU] Jakub Kuczmarski. *TeXUtilities package for Mathematica.* URL: https://github.com/jkuczm/MathematicaTeXUtilities.

Appendix A

Notation

A.1 'Equality up to' relations

Throughout this thesis identities are proven and investigated to varying degrees of accuracy. The following range of equalities will be used.

Relation	Meaning
$\overset{?}{=}$	Identity holds numerically to ≥ 500 decimal places on MZVs,
	or to ≥ 50 decimal places on MPLs
$\overset{\mathbb{Q}}{=}$	Identity holds up to a rational constant
$\overset{1}{=}$	The rational expected in $\overset{\mathbb{Q}}{=}$ is 1, numerically
$\overset{\mathcal{S}}{=}$	Identity holds on the level of the symbol
$\overset{⧢}{=}$	Identity holds for the symbol modulo products
$\overset{\delta}{=}$	Identity holds for the symbol modulo products and depth 1
$\overset{I_{3,2}}{=}$	Identity holds for the symbol modulo Li_5 and $I_{3,2}$ of 'simple' cross-ratios
$\overset{\delta^2}{=}$	Identity holds for the symbol modulo products and depth 2
$=$	Identity is known exactly

A.2 Symmetrised sums

Frequently we make use of sums over cyclic shifts of variables, sums over all permutations of variables, or alternating sums over all permutations. We introduce the following notation for these sums.

Sum over	Definition
All permutations	$\mathrm{Sym}_{\{ x_1,\ldots,x_n \}} f(x_1,\ldots,x_n) \coloneqq \sum_{\sigma\in S_n} f(x_{\sigma(1)},\ldots,x_{\sigma(n)})$
Signed permutations	$\mathrm{Alt}_{\{ x_1,\ldots,x_n \}} f(x_1,\ldots,x_n) \coloneqq \sum_{\sigma\in S_n} \mathrm{sgn}(\sigma) f(x_{\sigma(1)},\ldots,x_{\sigma(n)})$
Cyclic shifts	$\mathrm{Cyc}_{\{ x_1,\ldots,x_n \}} f(x_1,\ldots,x_n) \coloneqq \sum_{i=1}^{n} f(x_i,\ldots,x_n,x_1,\ldots,x_{i-1})$

Appendix B

Long weight 5 identities

B.1 Reducing $I_{3,2}$ to $I_{4,1}$ and Li_5 terms

Recall the 'brute force' identity in Identity 4.2.17, which expresses $I_{3,2}(x,y)$ in terms of $I_{4,1}$'s.

Identity 4.2.17. *Modulo δ, we can express the single term $I_{3,2}(x,y)$ using $I_{4,1}$ as follows.*

$$I_{3,2}(x,y) \overset{\delta}{=} -\frac{1}{2}\Big(3I_{4,1}(x,y) + I_{4,1}(x,\tfrac{1}{y}) + I_{4,1}(x,\tfrac{x}{y}) + \\ + I_{4,1}(x,\tfrac{y}{x}) - I_{4,1}(y,\tfrac{x}{y}) - I_{4,1}(y,\tfrac{y}{x})\Big)$$

This identity expressed $I_{3,2}(x,y)$ in terms of $I_{4,1}$'s, modulo δ. So it should then be possible to find Li_5 terms, which give an identity holding modulo products, on the nose. Indeed, we have the following identity, expressing $I_{3,2}(x,y)$ in terms of $I_{4,1}$'s and 141 Li_5 terms.

Identity B.1.1. *The following identity provides the missing Li_5 terms, which completes Identity 4.2.17 to an identity holding modulo $\sqcup\!\sqcup$. This gives us an expression for $I_{3,2}(x,y)$ in terms of $I_{4,1}$'s, and 141 Li_5 terms, modulo $\sqcup\!\sqcup$.*

$$\tfrac{22}{9}\Big(I_{3,2}(x,y) + \tfrac{1}{2}\Big(I_{4,1}(x,\tfrac{1}{y}) + I_{4,1}(x,\tfrac{x}{y}) + I_{4,1}(x,\tfrac{y}{x}) + 3I_{4,1}(x,y) - I_{4,1}(y,\tfrac{x}{y}) - I_{4,1}(y,\tfrac{y}{x})\Big)\Big) \overset{\sqcup\!\sqcup}{=}$$

$$\mathrm{Li}_5\Big(- \tfrac{23}{18}\left[\tfrac{1}{x}\right] + \tfrac{20}{3}\left[-\tfrac{1-x}{x}\right] + \tfrac{107}{54}\left[\tfrac{x}{y^2}\right] - \tfrac{103}{54}\left[\tfrac{1}{xy}\right] + \tfrac{1}{6}\left[\tfrac{x}{y}\right] - \tfrac{157}{54}\left[\tfrac{x^2}{y}\right] + 4\left[-\tfrac{1-y}{(1-x)y}\right]\Big) +$$

$$+ \tfrac{11}{3}\mathrm{Li}_5\Big([1-y] - \left[-\tfrac{1-x}{x(1-y)}\right] - \left[-\tfrac{1-y}{y}\right] - \left[\tfrac{x}{x-y}\right]\Big) - \tfrac{14}{3}\mathrm{Li}_5\Big(\left[\tfrac{x(x-y)}{(1-x)y}\right] + \left[-\tfrac{x-y}{(1-y)y}\right]\Big) +$$

$$+ 3\,\mathrm{Li}_5\Big(\left[\tfrac{(1-x)x}{x-y}\right] + \left[-\tfrac{x(1-y)}{y(x-y)}\right]\Big) - \tfrac{4}{3}\mathrm{Li}_5\Big(\left[-\tfrac{x-y}{(1-x)y}\right] + \left[\tfrac{x-y}{x(1-y)}\right]\Big) + \tfrac{7}{18}\mathrm{Li}_5\Big(\left[\tfrac{1}{y}\right] - \left[\tfrac{x(1-y)^2}{(1-x)^2y}\right]\Big) +$$

$$+ \tfrac{5}{18}\mathrm{Li}_5\Big(- \left[\tfrac{(x-y)^2}{(1-x)^2y}\right] - \left[\tfrac{(x-y)^2}{x(1-y)^2}\right]) + \tfrac{5}{27}\mathrm{Li}_5\Big(\left[-\tfrac{x^2(1-y)^3}{(1-x)^3y}\right] + \left[\tfrac{x(x-y)^3}{(1-x)^3y^2}\right] + \left[-\tfrac{(x-y)^3}{x(1-y)^3y}\right]\Big) +$$

$$+ \tfrac{8}{3}\mathrm{Li}_5\Big(\left[\tfrac{1-x}{1-y}\right] - \left[-\tfrac{1}{x-y}\right] - \left[-\tfrac{1-x}{y}\right] + \left[\tfrac{1-x}{y}\right] + \left[-\tfrac{x(1-y)}{y}\right] - \left[\tfrac{x(1-y)}{y}\right] + \left[\tfrac{x(1-y)}{y(x-y)}\right] + \\ - \left[-\tfrac{x-y}{(1-x)(1-y)}\right] + \left[-\tfrac{x-y}{y}\right]\Big) + \tfrac{2}{3}\mathrm{Li}_5\Big(\left[\tfrac{1}{x-y}\right] + \left[\tfrac{1-y}{(1-x)y}\right] - \left[-\tfrac{(1-y)(x-y)}{(1-x)y}\right] + \left[\tfrac{1-y}{x-y}\right] + \\ - \left[-\tfrac{x}{(1-x)y}\right] + \left[\tfrac{x(1-y)}{(1-x)y}\right] + \left[-\tfrac{x}{1-y}\right] - \left[\tfrac{x}{1-y}\right] + \left[\tfrac{x-y}{xy}\right]\Big) +$$

$$+\tfrac{5}{3}\,\mathrm{Li}_5\Big(-[1-x]-\Big[\tfrac{1-x}{x(1-y)}\Big]+\Big[-\tfrac{(1-x)x}{x-y}\Big]+\Big[-\tfrac{1-x}{x-y}\Big]-\Big[\tfrac{(1-x)(x-y)}{x(1-y)^2}\Big]-\Big[-\tfrac{(1-x)(x-y)}{x(1-y)}\Big]+$$
$$+\Big[\tfrac{(1-x)(x-y)}{x(1-y)}\Big]+\Big[\tfrac{(1-y)(x-y)}{(1-x)y}\Big]+\Big[\tfrac{x}{(1-x)y}\Big]-\Big[-\tfrac{x(1-y)(x-y)}{(1-x)^2y}\Big]-\Big[-\tfrac{x(x-y)}{(1-x)y}\Big]+$$
$$+\Big[\tfrac{x-y}{(1-x)(1-y)}\Big]-\Big[\tfrac{x-y}{(1-y)y}\Big]-\Big[-\tfrac{(x-y)^2}{(1-x)(1-y)y}\Big]-\Big[-\tfrac{x-y}{xy}\Big]\Big)+$$
$$+\tfrac{1}{9}\,\mathrm{Li}_5\Big(\Big[\tfrac{(1-x)(1-y)^3}{y(x-y)^2}\Big]-\Big[\tfrac{(1-x)^2(1-y)}{xy^2}\Big]-\Big[\tfrac{(1-x)^2x}{(1-y)y^2}\Big]+\Big[\tfrac{(1-x)^2(x-y)}{y^2}\Big]+\Big[\tfrac{(1-x)^2}{y^2(x-y)}\Big]+\Big[\tfrac{(1-x)^3}{x^2(1-y)(x-y)}\Big]+$$
$$+\Big[-\tfrac{(1-x)^3(x-y)}{x(1-y)^2}\Big]-\Big[-\tfrac{(1-x)x(1-y)^2}{y}\Big]-\Big[-\tfrac{1-x}{x^2(1-y)y}\Big]-\Big[-\tfrac{(1-x)x^2(1-y)}{y(x-y)^3}\Big]+\Big[\tfrac{(1-x)x^3}{y(x-y)}\Big]+$$
$$+\Big[\tfrac{(1-x)(x-y)}{(1-y)^3y}\Big]+\Big[\tfrac{(1-x)(x-y)^2}{x^3y}\Big]-\Big[-\tfrac{(1-x)(x-y)^3}{x(1-y)^2y}\Big]-\Big[\tfrac{(1-y)(x-y)^3}{(1-x)^2y^3}\Big]+\Big[\tfrac{x(1-y)^2(x-y)}{y^3}\Big]+$$
$$-\Big[-\tfrac{x(1-y)^3}{(1-x)^3y^2}\Big]+\Big[-\tfrac{x}{(1-y)(x-y)^2}\Big]-\Big[-\tfrac{x^2(1-y)^3}{(1-x)y^3(x-y)}\Big]-\Big[-\tfrac{x^2(1-y)^3}{y(x-y)^3}\Big]+\Big[-\tfrac{x^2(1-y)}{y^3(x-y)}\Big]+$$
$$-\Big[-\tfrac{x^3(1-y)^2}{(1-x)y^3}\Big]+\Big[\tfrac{x^3(1-y)^2}{y(x-y)}\Big]+\Big[\tfrac{x^3(1-y)(x-y)}{(1-x)^3y^2}\Big]-\Big[-\tfrac{x(x-y)}{(1-x)^2y^3}\Big]+\Big[-\tfrac{x(x-y)^2}{1-y}\Big]+\Big[\tfrac{(x-y)^2}{(1-x)^3(1-y)y}\Big]+$$
$$-\Big[\tfrac{(x-y)^2}{(1-x)x(1-y)^3}\Big]-\Big[\tfrac{(x-y)^3}{(1-x)^3xy}\Big]-\Big[-\tfrac{(x-y)^3}{(1-x)x^3(1-y)}\Big]\Big)+$$
$$+\tfrac{5}{9}\,\mathrm{Li}_5\Big(-\Big[\tfrac{1-x}{(1-y)^2}\Big]-\Big[\tfrac{(1-x)^2}{1-y}\Big]-\Big[\tfrac{(1-x)^2}{x(x-y)}\Big]+\Big[-\tfrac{(1-y)y}{(x-y)^2}\Big]-\Big[-\tfrac{x^2}{(1-x)(x-y)}\Big]-\Big[-\tfrac{x^2(1-y)}{(1-x)^2y}\Big]+$$
$$+\Big[-\tfrac{x-y}{(1-x)y^2}\Big]+\Big[\tfrac{(x-y)^2}{(1-x)y^2}\Big]+\Big[\tfrac{(x-y)^2}{x^2(1-y)}\Big]+\Big[\tfrac{x-y}{x(1-y)^2}\Big]\Big)+$$
$$+\mathrm{Li}_5\Big(\Big[\tfrac{1}{x(1-y)}\Big]+\Big[-\tfrac{(1-x)(1-y)}{y}\Big]-\Big[\tfrac{1-x}{(1-y)y}\Big]-\Big[\tfrac{(1-x)(1-y)}{y(x-y)}\Big]-\Big[-\tfrac{(1-x)^2}{x(1-y)}\Big]-\Big[-\tfrac{1-x}{x(x-y)}\Big]+$$
$$-\Big[\tfrac{(1-x)(x-y)}{1-y}\Big]+\Big[-\tfrac{(1-x)(x-y)}{(1-y)y}\Big]+\Big[-\tfrac{1-x}{xy}\Big]-\Big[\tfrac{(1-x)x}{y}\Big]+\Big[-\tfrac{(1-x)x}{y(x-y)}\Big]-\Big[\tfrac{(1-x)(x-y)}{xy}\Big]+$$
$$+\Big[-\tfrac{(1-y)(x-y)}{(1-x)^2y}\Big]+\Big[\tfrac{x(1-y)}{(1-x)y^2}\Big]+\Big[\tfrac{x(1-y)^2}{(1-x)y(x-y)}\Big]+\Big[-\tfrac{x(1-y)^2}{y(x-y)}\Big]+\Big[-\tfrac{x(1-y)(x-y)}{(1-x)y^2}\Big]-\Big[-\tfrac{x(1-y)}{y^2}\Big]+$$
$$-\Big[\tfrac{x^2(1-y)}{(1-x)y}\Big]+\Big[\tfrac{x^2(1-y)}{y(x-y)}\Big]-\Big[\tfrac{x^2}{x-y}\Big]-\Big[\tfrac{x(x-y)}{(1-x)^2y}\Big]+\Big[-\tfrac{x-y}{(1-x)(1-y)y}\Big]-\Big[\tfrac{x-y}{(1-x)x(1-y)}\Big]+$$
$$-\Big[\tfrac{x-y}{(1-y)^2}\Big]+\Big[-\tfrac{(x-y)^2}{(1-x)x(1-y)}\Big]+\Big[-\tfrac{(x-y)^2}{(1-x)xy}\Big]+\Big[\tfrac{(x-y)^2}{x(1-y)}\Big]-\Big[\tfrac{x}{y(x-y)}\Big]-\Big[-\tfrac{y}{(1-y)(x-y)}\Big]\Big)+$$
$$+\tfrac{4}{9}\,\mathrm{Li}_5\Big(\Big[\tfrac{1}{(1-x)(1-y)}\Big]+\Big[\tfrac{(1-x)(1-y)}{xy}\Big]+\Big[\tfrac{(1-x)x}{(1-y)y}\Big]+\Big[-\tfrac{(1-x)x}{(x-y)^2}\Big]-\Big[-\tfrac{(1-x)(x-y)}{y}\Big]-\Big[-\tfrac{1-x}{y(x-y)}\Big]+$$
$$-\Big[-\tfrac{(1-y)^2}{y(x-y)}\Big]+\Big[-\tfrac{x(1-y)^2}{(1-x)y^2}\Big]-\Big[\tfrac{x}{(1-y)(x-y)}\Big]+\Big[\tfrac{x^2(1-y)}{(1-x)y^2}\Big]-\Big[\tfrac{x(x-y)}{1-y}\Big]-\Big[-\tfrac{x-y}{(1-x)^2y}\Big]+$$
$$-\Big[\tfrac{x-y}{x^2(1-y)}\Big]-\Big[\tfrac{y^2}{(1-y)(x-y)}\Big]\Big)$$

Remark B.1.2. The candidate Li_5 arguments which eventually produced this identity were generated using Radchenko's sage package MESA [MESA], and the `set_extra_primes_tree_search` routine. This allows a good choice of extra factors to appear in $1-\alpha$, when computing the symbol of $\mathrm{Li}_n(\alpha)$. For example, even though the factor $-x+x^2-xy+y^2$ does not appear anywhere in the symbol of the left hand side of Identity B.1.1, it does appear in the symbol of the following Li_5 terms on the right hand side.

$$-\tfrac{1}{9}\Big[\tfrac{(1-x)^2x}{(1-y)y^2}\Big]-\tfrac{1}{9}\Big[-\tfrac{(1-x)x^2(1-y)}{y(x-y)^3}\Big]+\Big[-\tfrac{(1-x)(x-y)}{(1-y)y}\Big]-\tfrac{1}{9}\Big[-\tfrac{(1-x)(x-y)^3}{x(1-y)^2y}\Big]+\Big[-\tfrac{(1-x)x}{y(x-y)}\Big]+\Big[\tfrac{(x-y)^2}{x(1-y)}\Big]\,.$$

But somehow, they conspire to cancel in just the right way as to make this factor disappear in the end. Because of this phenomenon, and the large number of potential arguments otherwise, finding Identity B.1.1 would potentially be very difficult if not for the MESA software [MESA].

B.2 Relating depth 3 iterated integrals

Recall Theorem 4.3.18, which claimed that modulo $I_{3,2}$ all depth 3 iterated integrals are somehow 'equivalent'.

Theorem 4.3.18. *Modulo $I_{3,2}$, all of the weight 5, depth 3 iterated integrals span the same space. More precisely, if*

$$\mathcal{B}_f \coloneqq \left\{ f(\sigma \cdot abcdef) \mid \sigma \in S_{\{ a,b,c,d,e,f \}} \right\} ,$$

then $\operatorname{span} \mathcal{B}_f$*, modulo $I_{3,2}$, is invariant for $f \in \{ I_{3,1,1}, I_{1,3,1}, I_{1,1,3}, I_{2,2,1}, I_{2,1,2}, I_{1,2,2} \}$.*

The proof was to give the relevant identities expressing each depth 3 integral $I_{n_1,n_2,n_3}(abcdef)$ as a sum of other depth 3 integrals, modulo $I_{3,2}$. The short identities relating $I_{3,1,1}$ and $I_{1,3,1}$, relating $I_{3,1,1}$ and $I_{1,1,3}$, and expressing $I_{2,2,1}$ as a sum of $I_{3,1,1}$'s were given already in the proof. The remaining identities are presented below.

The following three identities express $I_{3,1,1}(abcdef)$ as a sum of $I_{2,1,2}$'s, express $I_{2,1,2}(abcdef)$ as a sum of $I_{1,2,2}$'s, and express $I_{1,2,2}(abcdef)$ as a sum of $I_{2,2,1}$'s modulo $I_{3,2}$. With these identities the proof of Theorem 4.3.18 is complete.

Identity B.2.1. *The following identity expresses $I_{3,1,1}(abcdef)$ as a sum of 197 $I_{2,1,2}$ terms and 24 $I_{3,2}$, modulo δ.*

$$\begin{aligned}
12 I_{3,1,1}(abcdef) \overset{\delta}{=} I_{2,1,2}\big(&2[abcdfe] - [abdcfe] + [abdfec] - [abfcde] + [abfdce] + \\
&+ [acbdfe] - [acbefd] + [acdbef] + [acdfeb] - [acedbf] - [acfbde] - [acfbed] - [acfedb] + \\
&+ [adbecf] + [adbefc] + [adcbfe] - [adcfeb] + [adebfc] + [adefbc] + [adefcb] - [adfcbe] + \\
&- [adfecb] + [aebcfd] - [aebdcf] + [aebfcd] - [aecbfd] + [aecdfb] + [aedcfb] + [aedfbc] + \\
&+ [aedfcb] + [aefbcd] - [afbcde] - [afbdec] + [afcdbe] - [afcedb] + [afdcbe] - [afdecb] + \\
&+ [afebdc] + [afedbc] - [bacfde] - [badfec] - [baecdf] + [baefdc] + [bafcde] + [bafdec] + \\
&+ [bafecd] + [bcadfe] - [bcaefd] + [bcdaef] - [bcedaf] + [bcedfa] - [bcefad] - [bcfeda] + \\
&+ [bdcefa] + [bdeafc] + [bdecaf] + [bdefca] - [bdface] - [bdfaec] - [beadfc] - [becadf] + \\
&- [becdfa] + [bedacf] + [bedcfa] + [befacd] + [bfadce] + [bfaecd] - [bfcaed] + [bfdcea] + \\
&+ [bfdeca] + [bfeadc] + [cabdfe] - [cabfde] - [cadbef] - [caefbd] + [cafdeb] + [cafebd] + \\
&- [cbafde] - [cbdefa] - [cbdfae] - [cbeafd] + [cbfdae] + [cbfeda] - [cdabef] - [cdabfe] + \\
&- [cdbeaf] - [cdbefa] + [cdbfae] - [cdbfea] + [cdeabf] + [cdeafb] - [cdfabe] - [cdfaeb] + \\
&- [cebdaf] - [cebdfa] - [cebfda] + [cedabf] + [cedbaf] + [cedfab] + [cefbad] - [cfadeb] + \\
&- [cfbdae] - [cfbdea] - [cfdbea] - [cfdeab] - [cfdeba] + [cfebad] + [cfebda] + [dacefb] + \\
&- [daebfc] - [daecbf] - [dbaefc] - [dbcefa] - [dbecfa] + [dbfaec] + [dbfcea] + [dcabfe] + \\
&+ [dcafeb] - [dceafb] - [dcebaf] - [dcebfa] + [dcfaeb] - [deabcf] + [deacbf] - [deafbc] + \\
&+ [debfca] - [decafb] - [decbfa] - [decfab] - [decfba] + [defbca] + [dfabec] + [dfaecb] +
\end{aligned}$$

$$+ [dfbaec] - [dfbcea] + [dfbeca] - [dfcbae] - [dfcbea] - [dfebac] - [dfebca] - [eabcfd] +$$
$$+ [eacbfd] - [eacdfb] + [eacfdb] - [eadbfc] - [eadcbf] - [eadcfb] + [ebcadf] + [ebcfda] +$$
$$- [ebdafc] + [ecadfb] + [ecafbd] - [ecdbaf] - [edbcaf] + [edcafb] + [edcbfa] - [edfabc] +$$
$$- [edfacb] - [edfbca] - [edfcab] - [efadcb] + [efbcad] + [efbdac] + [efbdca] + [efcabd] +$$
$$- [efdabc] - [efdacb] - [efdbca] - [efdcba] - [fabdce] + [fabecd] - [fadcbe] + [fadceb] +$$
$$- [faecdb] - [fbaced] - [fbaedc] - [fbeadc] - [fbecda] - [fbedac] - [fbedca] + [fcadbe] +$$
$$+ [fcbade] - [fcbeda] + [fcdbea] + [fcdeab] + [fcdeba] - [fceabd] + [fdacbe] + [fdceab] +$$
$$+ [fdebac] + [fdecab] - [feabdc] - [feacdb] - [feadbc] - [fecbda] + [fedcab] + [fedcba]\big)+$$

$$+ I_{3,2}\big([abcde] - [abcef] + [abcfe] - [abfed] - [acbdf] + [acbed] - [acfbe] - [adbcf] +$$
$$- [adfcb] + [aebdf] - [aecfb] + [bafce] + [bafed] - [bcade] + [bcdaf] + [bdace] +$$
$$- [bdfac] - [beacf] - [becfa] - [bfadc] + [bfaed] - [cabed] - [cdabf] - [cdfab]\big)\,.$$

Identity B.2.2. *The following identity expresses $I_{2,1,2}(abcdef)$ as a sum of 230 $I_{1,2,2}$ terms, and 1 $I_{3,2}$ term, modulo δ.*

$$3I_{2,1,2}(abcdef) \overset{\delta}{=} I_{1,2,2}\big([abcdef] - [abcdfe] - [abcedf] - [abdcef] + [abdcfe] + [abdefc] +$$
$$+ [abecdf] - [abecfd] - [abefcd] - [abfcde] - [abfdce] + [abfdec] + [abfecd] - [abfedc] +$$
$$- [acbdef] - [acbedf] + [acbefd] - [acbfed] + [acdbef] - [acdebf] + [acdefb] - [acebfd] +$$
$$+ [acedfb] + [acefbd] + [acefdb] - [acfbde] + [acfbed] + [acfebd] - [adbcef] - [adbecf] +$$
$$+ [adbefc] + [adcbef] - 2[adcbfe] + [adcebf] + [adcefb] + [adcfbe] - [adebfc] + [adecfb] +$$
$$- [adefbc] + [adfbce] + [adfbec] - [adfcbe] + 2[adfceb] + [adfebc] - [adfecb] - [aebcdf] +$$
$$+ [aebcfd] - [aecbfd] + [aecdfb] - [aecfdb] + [aedbfc] + [aedfbc] + [aefbcd] - [aefcdb] +$$
$$+ [aefdbc] - [aefdcb] + [afbced] - [afbdce] + [afbdec] + [afbecd] + [afbedc] + [afcbed] +$$
$$- [afcdbe] - [afcdeb] - [afcedb] - [afdbce] - 2[afdcbe] + [afdceb] + [afdecb] + [afebdc] +$$
$$+ [afecbd] - 2[bacdef] + [bacedf] - [bacfed] + [badcef] - [badcfe] - [badfce] + [baecfd] +$$
$$+ [baefcd] + [bafced] + 2[bafdce] + [bcadef] + [bcadfe] + [bcaedf] - [bcaefd] - [bcdaef] +$$
$$+ [bcdafe] - [bcdeaf] + [bcdfae] - [bcdfea] - [bcedaf] - [bcfade] + [bcfdae] - [bdafec] +$$
$$+ [bdcaef] - [bdceaf] + [bdcefa] + [bdcfae] + [bdcfea] - [bdeafc] - [bdecfa] + [beacfd] +$$
$$- 2[beadfc] + [beafcd] - [beafdc] + [becadf] + [becdfa] + [becfad] - [becfda] - [bedacf] +$$
$$+ [bedafc] - [bedcfa] + [bedfac] + [befacd] - [befadc] + [befdac] - [befdca] - [bfacde] +$$
$$- [bfaced] + [bfadec] + [bfcade] + [bfcaed] + [bfceda] - [bfdaec] + [bfdcae] + [bfdcea] +$$
$$- [bfdeca] - [bfeadc] + [bfecda] - [bfedac] + [cabdfe] - [cabefd] + [cadfbe] - [caebdf] +$$
$$+ [caebfd] - [caefdb] - [cafbed] - [cafdeb] - [cafebd] - [cafedb] - [cbadef] + [cbdefa] +$$
$$- [cbdfae] - [cbeafd] + 2[cbedaf] - [cbedfa] - 2[cbefad] + [cbefda] + [cbfaed] - [cbfdae] +$$

$$- [cbfdea] + [cbfead] - [cbfeda] - [cdbaef] - [cdbeaf] - [cdeabf] + [cdeafb] - [cdebfa] +$$
$$- [cdefba] + [cdfeab] + [ceafdb] - [cebadf] - [cebfad] + [cedabf] - [cedbfa] - [cedfab] +$$
$$- [cefabd] + [cefadb] - [cefbda] + [cfabde] - [cfbdea] - [cfbeda] + [cfdabe] - [cfdaeb] +$$
$$- [cfdeab] - [cfeabd] - [cfebad] + [cfedab] + [dabcef] + [dabcfe] - [dacbef] + [dacbfe] +$$
$$+ [daecbf] - [dafbce] - [dafbec] - [dafceb] - 2[dafebc] + [dafecb] - [dbacef] - [dbacfe] +$$
$$+ [dbcafe] - [dbcefa] - [dbeacf] + [dbeafc] + [dbefac] - [dbefca] - [dbface] + 2[dbfaec] +$$
$$+ [dbfcae] + [dbfeac] - [dcafbe] + [dcafeb] - [dcbafe] - [dcebaf] - [dcfabe] + [dcfbae] +$$
$$- [deacbf] - [deacfb] - [deafcb] + [debacf] + [debcaf] + [decfab] + [defbac] - [defbca] +$$
$$+ [dfaecb] - [dfbeac] + [dfcaeb] - [dfeabc] - [dfebca] + [eabcfd] + [eabfcd] - [eafbdc] +$$
$$- [ebacdf] - [ebadcf] + [ebcdfa] + [ebdcfa] - [ecbadf] - [ecdfab] - [edcabf] - [efadbc]\big)+$$
$$- I_{3,2}(abcde)\,.$$

Identity B.2.3. *The following identity expresses $I_{1,2,2}(abcdef)$ as a sum of 177 $I_{2,2,1}$ terms, and 1 $I_{3,2}$ term, modulo δ.*

$$I_{1,2,2}(abcdef) \overset{\delta}{=} I_{2,2,1}\big([abcfde] + [abdcfe] - [abecfd] - [abefcd] + [abfcde] - [abfced] +$$
$$- [abfecd] + [acbdef] - [acdbfe] - [acdebf] + [acefdb] - [acfbde] - [acfdbe] - [adbcfe] +$$
$$+ [adbfec] + [adcfeb] - [adfcbe] + [adfceb] + [aebcfd] + [aebdfc] + [aebfdc] - [aedbcf] +$$
$$- [aedfcb] + [aefdbc] - [aefdcb] + [afbcde] + [afbced] + [afcdeb] - [afdbce] - [afdcbe] +$$
$$- [afebcd] - [afecdb] - [afedbc] + [bacdfe] - [bacfde] + [bacfed] + [baecfd] + [baefcd] +$$
$$- [baefdc] - [bafedc] + [bcefda] + [bdacef] - [bdaefc] + [bdafce] - [bdcefa] + [bdcfae] +$$
$$+ [bdecaf] - [bdecfa] + [becfda] - [bfaced] - [bfadce] + [cabdfe] + [cabefd] + [cabfde] +$$
$$- [cadbef] + [cadfbe] - [cadfeb] - [caebfd] - [caefdb] + [cafbde] + [cafedb] - [cbdfea] +$$
$$+ [cbfade] - [cdabef] + [cdafbe] + [cdbeaf] + [cdbefa] + [cdbfae] - [cdefba] + [cdfeab] +$$
$$- [cdfeba] - [ceadfb] + [ceafbd] - [cebafd] + [cebdaf] - [cedabf] - [cedafb] - [cedbfa] +$$
$$- [cefadb] + [cefbad] - [cefdba] + [cfabde] - [cfadbe] + [cfbade] + [dabcfe] + [dabefc] +$$
$$- [dabfec] + [dacbef] + [dacfbe] - [daebfc] - [daecbf] - [daecfb] - [dafceb] - [dbaecf] +$$
$$+ [dbaefc] - [dbafec] + [dbcaef] + [dbcafe] - [dbceaf] + [dbcfea] + [dbeacf] - [dbecaf] +$$
$$- [dbefac] - [dcafbe] + [dcafeb] + [dcbaef] + [dcbafe] - [dcbeaf] + [dcbfea] + [dceabf] +$$
$$- [dcebfa] + [dcefab] - [dcfabe] - [dcfbea] + [deafcb] - [debfac] + [debfca] + [decabf] +$$
$$- [decafb] + [decbaf] - [decbfa] - [defacb] - [defbca] - [defcba] + [dfacbe] - [dfbace] +$$
$$- [dfbaec] + [dfbeac] + [dfcabe] + [dfcbae] - [dfcbea] - [dfeacb] - [dfebca] - [eabdfc] +$$
$$- [eabfdc] + [eacfbd] + [eacfdb] - [eadbfc] - 2[eafcbd] - [eafdbc] - [ebdacf] - [ebfacd] +$$
$$- [ebfcad] - [ecabfd] + [ecafbd] - [ecafdb] + [ecbadf] + [ecbdfa] - [ecdfab] + [ecdfba] +$$

$$+ [ecfabd] + [edacbf] - [edacfb] + [edbacf] + [edcabf] + [edcbfa] - [edfabc] - [edfbac] +$$
$$+ [edfbca] + [efabdc] - [efacbd] - [efbdac] - [efbdca] + [fabdec] - [facedb] - [fadecb] +$$
$$- [faecdb] - [faedcb] - [fcabde] - [fcadeb] + [fcaebd] - [fdabec] + [fdacbe] - [fdaecb] +$$
$$- [feabdc] + [feacbd] - [feadcb]\big) +$$
$$- I_{3,2}(abedf) \,.$$

B.3 Dan's reduction for $I_{1,1,1,1,1}$

In Section 5.3 we applied Dan's reduction procedure to $I_{1,1,1,1,1}$ and produced an expression for $I_{1,1,1,1,1}$ in terms of the 11 depth ≤ 3 integrals $I_5, I_{4,1}, \ldots, I_{1,4}, I_{3,1,1}, \ldots, I_{1,2,2}$. In Section 5.3.2 we indicated that identities from Chapter 4 could be used to reduce $I_{1,1,1,1,1}$ explicitly to $I_{3,1,1}$, $I_{3,2}$ and I_5 terms modulo products. The following theorem shows this reduction explicitly.

Theorem B.3.1. *As shorthand recall the 'coupled cross-ratio' notation* $I_{n_1,\ldots,n_k}(abcd_1 \ldots d_k) \coloneqq I_{n_1,\ldots,n_k}(\mathrm{cr}(a,b,c,d_1),\ldots,\mathrm{cr}(a,b,c,d_k))$ *from Section 4.1.2. Then modulo products, we can give the following identity for* $I_{1,1,1,1,1}$.

$$[a \mid b,c,d,e,f \mid g] = \psi'(a;b,c,d,e,f) - \psi'(g;b,c,d,e,f)\,,$$

where

$$\psi'(a;b,c,d,e,f) \coloneqq$$
$$I_{3,1,1}(-[bdacef] + [bdae\infty c] - [bdaf\infty c] + [bda\infty ef] + [bdcae\infty] + [bdca\infty e] + [bdc\infty ae] +$$
$$+ [bde\infty af] + [bd\infty aef] + [bd\infty eaf] - [bfac\infty e] + [bfad\infty e] - [bfa\infty ce] + [bfa\infty dc] +$$
$$+ [bfa\infty de] - [bfa\infty ec] + [bfcad\infty] - [bfcaed] - [bfcae\infty] + [bfca\infty d] + [bfcda\infty] +$$
$$- [bfcea\infty] + [bfda\infty e] - [bfeca\infty] + [bfeda\infty] - [d\infty acbf] + [d\infty aceb] + [d\infty acef] +$$
$$- [d\infty acfb] + [d\infty aebc] + [d\infty aecb] - [d\infty afbc] - [d\infty afcb] + [d\infty bcae] + [d\infty cabe] +$$
$$+ [d\infty cbae] + [d\infty ebaf] - [f\infty abce] + [f\infty abdc] + [f\infty abde] - [f\infty abec] - [f\infty acbe] +$$
$$- [f\infty aceb] + [f\infty adbe] + [f\infty adeb] + [f\infty caed] + [f\infty dabe] + [f\infty daeb] + [f\infty deab] +$$
$$- [\infty bacdf] + [\infty baced] - [\infty bacfd] - [\infty bacfe] + [\infty badef] + [\infty badfe] + [\infty baecd] +$$
$$+ [\infty baedc] - [\infty bafcd] - [\infty bafce] + [\infty bafde] - [\infty bafec] + [\infty bcade] + [\infty bcaed] +$$
$$+ [\infty bcdae] + [\infty bdaef] + [\infty bdafe] + [\infty bdcae] + [\infty bdeaf] + [\infty bedaf]) +$$
$$+ I_{3,2}([bdace] - [bdae\infty] + [bda\infty f] + [bde\infty c] + [bde\infty f] + 2[bd\infty ae] + [bd\infty af] +$$
$$+ [bd\infty ec] + [bd\infty ef] + [bfad\infty] + [bfa\infty c] - 2[bfa\infty d] + [bfa\infty e] - [bfca\infty] +$$
$$- [bfce\infty] + 3[bfda\infty] + [bfde\infty] + [bfd\infty c] - [bfec\infty] - [bfe\infty d] + [bf\infty dc] +$$
$$- [bf\infty ed] + [b\infty cad] + [b\infty cae] + [b\infty dae] + [b\infty daf] + [dbeaf] + 2[db\infty ae] +$$

$$+ [d\infty abe] - [d\infty aeb] - [d\infty aec] + [d\infty aef] + 3[d\infty bae] + [d\infty baf] + [d\infty bce] +$$
$$+ [d\infty bef] + [d\infty cae] + [d\infty cbe] - [d\infty efa] - [d\infty efb] - [d\infty feb] - [fbcae] +$$
$$+ [fbdae] + 2[fbda\infty] - 2[fbea\infty] - [f\infty abd] + [f\infty aeb] + [f\infty bed] + 2[f\infty eab] +$$
$$+ [f\infty ebd] - [\infty baec] - [\infty baed] + 2[\infty baef] - [\infty bafd] + [\infty bcae] + [\infty bcde] +$$
$$+ [\infty bdaf] + [\infty bdef] + 2[\infty beaf] - [\infty befa] + 2[\infty dbae] + [\infty dbaf] + [\infty dcab] +$$
$$- [\infty deaf] + [\infty fcae] - [\infty fdae] + [\infty feab]) +$$
$$+ \frac{1}{3} I_{3,2}(-[bdacf] + 4[bdaef] - [bdafc] - 2[bdafe] - [bdca\infty] - [bdc\infty a] + 7[bdeaf] +$$
$$- 2[bdefa] - [bfade] - [bfae\infty] - [bfcad] - [bfcda] + 2[bfdae] - [bfdce] +$$
$$+ 2[bfdea] - 7[bfea\infty] + 5[bfed\infty] - [bfe\infty a] - [b\infty dea] - [b\infty dec] + [b\infty eda] +$$
$$- [b\infty efa] - [b\infty efd] + [b\infty fea] + [d\infty acf] + [d\infty afc] - [d\infty afe] + 4[d\infty ebf] +$$
$$+ [fbdea] + [fbdec] - [fbeda] - 2[fbe\infty a] - 2[fbe\infty d] + 2[fb\infty ea] + [f\infty abc] +$$
$$+ [f\infty acb] + [f\infty ade] + [f\infty cad] + [f\infty cda] - 2[f\infty dae] + [f\infty dce] - 2[f\infty dea] +$$
$$+ 2[\infty bacf] + 4[\infty bade] + 2[\infty bafc] - [\infty bafe] + [\infty bcad] + [\infty bcda] + 7[\infty bdae] +$$
$$+ 4[\infty bdce] - 2[\infty bdea] + 4[\infty bedf] - [\infty defa] - [\infty defb] + [\infty dfea] - [\infty fdea] +$$
$$- [\infty fdec] + [\infty feda]) +$$
$$+ I_5(-[bdac] + 15[bdae] + 15[bdaf] - 2[bda\infty] + 6[bdce] + 5[bdc\infty] + 13[bdef] + 6[bd\infty e] +$$
$$+ 6[bd\infty f] - 3[bfad] + 8[bfae] - 8[bfa\infty] - 2[bfce] - 8[bfde] + 10[bfd\infty] - 8[bfea] +$$
$$+ 3[d\infty ab] + 21[d\infty ae] - 3[d\infty af] + 2[d\infty bf] + 6[d\infty ce] + 13[f\infty ab] + [f\infty ad] +$$
$$- 7[f\infty ae] + 2[f\infty ce] + 6[f\infty db] + 6[f\infty eb] + 4[\infty bad] + 14[\infty bae] + 10[\infty baf] +$$
$$+ 8[\infty bce] + 13[\infty bde] + 8[\infty bdf] + 4[\infty bea]) +$$
$$+ \frac{1}{3} I_5(19[bfcd] + 4[bfda] - 13[bfe\infty] + 32[bf\infty a] + 23[d\infty be] - 4[d\infty ea] +$$
$$+ 22[d\infty ef] + 16[d\infty fa] - [f\infty cd] - 4[f\infty da] + 16[f\infty de] + 16[f\infty ea] - [\infty bcd] +$$
$$- 4[\infty bda] + 40[\infty bef] + 16[\infty bfa]) \,.$$

Appendix C

Proof of the $I^-_{4,1}(x, \Sigma_i [p_i])$ identity

C.1 Statement of the theorem

Firstly, let us recall the identity we intend to prove using symbol.

Theorem 7.4.6. *For $I^-_{4,1}$ applied to the* Li_2 *algebraic equation, we can find explicit* Li_5 *terms, and give the following identity.*

$$
\begin{aligned}
&I^-_{4,1}(x, \textstyle\sum_i [p_i]) \overset{\text{ш}}{=} \\
&\quad -\frac{c}{2}\,\mathrm{Li}_5(x) + b\,\mathrm{Li}_5(1-x) + b\,\mathrm{Li}_5(1-\tfrac{1}{x}) + && \text{(7.4.5a)} \\
&\quad + \mathrm{Li}_5^{\rho^-}\left(\frac{1}{abc(c-a))}\left[\frac{t}{g(p,x)}\right]\right) + \sum_{p\in\{\,p_i\,\}} \mathrm{Li}_5^{\rho^-}\left(-\frac{b}{8(c-a)}\left[\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right] + \right. && \text{(7.4.5b)} \\
&\quad \left. + \left(\frac{c-a}{4b}+1\right)[xp_i] + \frac{b}{a}\left(\left[\frac{1}{1-p_i}\right] - \left[\frac{1-x}{1-p_i}\right] - \left[\frac{1-1/x}{1-p_i}\right]\right)\right) && \text{(7.4.5c)}
\end{aligned}
$$

Here $I^-_{4,1}$ is as in Definition 7.4.1, and $\mathrm{Li}_5^{\rho^-}$ is the symmetrisation we obtain using Definition 7.3.11 and the automorphism ρ from Definition 7.4.5. We assume $a, b > 0$, and define c by $a + b + c = 0$. Moreover t is as in Equation 7.3.1, defining the p_i, and $g(\alpha, x)$ is as in Definition 7.3.10.

The first step, before we begin the proof, is to give the full expanded out version of this identity. This is so that all the terms are immediately visible, and we can calculate directly the symbol. Also, since $I^-_{4,1}$ is defined with a factor of $\frac{1}{2}$, it may be marginally more convenient to multiply by 2 throughout, rather than carry factors of $\frac{1}{2}$ through the calculation of the symbol of $I_{4,1}$. So the version of the theorem we will prove is the following.

Theorem C.1.1. *For $I^-_{4,1}$ applied to the* Li_2 *algebraic equation, we can find explicit* Li_5 *terms, and give the following identity.*

$$
\begin{aligned}
&I_{4,1}(x, \textstyle\sum_i [p_i]) - I_{4,1}(x, \sum_i [\frac{1}{p_i}]) \overset{\text{ш}}{=} \\
&\quad -c\,\mathrm{Li}_5(x) + 2b\,\mathrm{Li}_5(1-x) + 2b\,\mathrm{Li}_5(1-\tfrac{1}{x}) + && \text{(C.1.1a)}
\end{aligned}
$$

$$+\frac{2}{abc(c-a))}\,\mathrm{Li}_5\left(\left[\frac{t}{x^a(1-x)^b}\right]+\left[\frac{t}{x^c(x-1)^b}\right]\right)+ \tag{C.1.1b}$$

$$+\sum_i\Bigg\{-\frac{b}{2(c-a)}\,\mathrm{Li}_5\left(\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right)+ \tag{C.1.1c}$$

$$+\left(\frac{c-a}{2b}+2\right)\mathrm{Li}_5\left(xp_i\right)+\left(\frac{c-a}{2b}-2\right)\mathrm{Li}_5\left(\frac{x}{p_i}\right)+ \tag{C.1.1d}$$

$$+\frac{2b}{a}\,\mathrm{Li}_5\left(\left[\frac{1}{1-p_i}\right]-\left[\frac{1-x}{1-p_i}\right]-\left[\frac{1-1/x}{1-p_i}\right]\right)+ \tag{C.1.1e}$$

$$-\frac{2b}{c}\,\mathrm{Li}_5\left(\left[\frac{1}{1-1/p_i}\right]-\left[\frac{1-x}{1-1/p_i}\right]-\left[\frac{1-1/x}{1-1/p_i}\right]\right)\Bigg\}. \tag{C.1.1f}$$

C.2 Proof of the theorem

This theorem is proven by directly computing and comparing the symbol of both sides. I will break this down into a number of easier to understand steps.

C.2.1 Symbol of the right hand side

Let's compute the symbol of the RHS of Equation C.1.1, and gather by the last tensor factor initially. We know that $\mathcal{S}(\mathrm{Li}_5(\alpha)) \overset{\sqcup\!\sqcup}{=} -(1-\alpha)\wedge\alpha\otimes\alpha^{\otimes 3}$. We shall write $\{\alpha\}_n = -(1-\alpha)\wedge\alpha\otimes\alpha^{n-2}$, so that we may write the symbol of $\mathrm{Li}_5(\alpha)$ as $\{\alpha\}_4\otimes\alpha$ or $\{\alpha\}_3\otimes\alpha\otimes\alpha$ for simplicity.

Equation C.1.1a: The symbol of this is

$$-c\,\{x\}_4\otimes x+2b\,\{1-x\}_4\otimes(1-x)+2b\,\{1-1/x\}_4\otimes(1-1/x)$$

Now expand out $\otimes(1-1/x)=\otimes(1-x)-\otimes x$ to get

$$\begin{aligned}\mathcal{S}(\text{Equation C.1.1a}) = {}& -\left(c\,\{x\}_4+2b\,\{1-1/x\}_4\right)\otimes x+\\ &+\left(2b\,\{1-x\}_4+2b\,\{1-1/x\}_4\right)\otimes(1-x)\,.\end{aligned}$$

Equation C.1.1b: The symbol of this is

$$\frac{2}{abc(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_4\otimes\frac{t}{x^a(1-x)^b}+\frac{2}{abc(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_4\otimes\frac{t}{x^c(x-1)^b}$$

Since $t=\pm\prod_j p_j$, and ±1 is irrelevant in the symbol, we have that $\otimes\frac{t}{x^a(1-x)^b}=\otimes\frac{\prod_j p_j}{x^a(1-x)^b}=\otimes\left(\sum_j[p_j]-a[x]-b[1-x]\right)$. So we obtain

$$\begin{aligned}\mathcal{S}(\text{Equation C.1.1b}) = {}& \frac{2}{abc(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_4\otimes\left(\textstyle\sum_i[p_i]-a[x]-b[1-x]\right)+\\ &+\frac{2}{abc(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_4\otimes\left(\textstyle\sum_i[p_i]-c[x]-b[1-x]\right).\end{aligned}$$

Equation C.1.1d: The symbol of this is

$$\sum_i \left(\frac{c-a}{2b}+2\right)\{xp_i\}_4 \otimes (xp_i) + \left(\frac{c-a}{2b}-2\right)\left\{\frac{x}{p_i}\right\}_4 \otimes \frac{x}{p_i}\,,$$

which expands out to give

$$\begin{aligned}\mathcal{S}(\text{Equation C.1.1d}) = &\sum_i (\tfrac{c-a}{2b}+2)\{xp_i\}_4 \otimes ([x]+[p_i]) + \\ &+\sum_i (\tfrac{c-a}{2b}-2)\left\{\frac{x}{p_i}\right\}_4 \otimes ([x]-[p_i])\,.\end{aligned}$$

Remark C.2.1. In the remaining terms we will need to use the result that

$$1-p_i = \pm\frac{\prod_j p_j^{1/b}}{p_i^{a/b}}\,,$$

since the p_i are roots of the equation $x^a(1-x)^b = t$. Doing this does assume that $a, b > 0$, in order to have $\prod p_j = \pm t$. This allows us to eliminate $1-p_i$ factors in favour of p_i factors in the symbol.

Equation C.1.1c: The symbol is

$$\sum_i -\frac{b}{2(c-a)}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_4 \otimes \frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\,.$$

Using the above, we find the last factor expands out to

$$\otimes(2[1-x]-[x]+[p_i]-2[1-p_i])\,,$$

and that $1-p_i$ further expands out to

$$\otimes(\tfrac{1}{b}\textstyle\sum_j [p_j] - \tfrac{a}{b}[p_i])\,,$$

giving overall

$$\otimes(2[1-x]-[x]+[p_i]-\tfrac{2}{b}\textstyle\sum_j [p_j] + \tfrac{2a}{b}[p_i])\,.$$

So

$$\begin{aligned}\mathcal{S}(\text{Equation C.1.1c}) = &\sum_i -\frac{b}{2(c-a)}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_4 \otimes \\ &\otimes (2[1-x]-[x]+[p_i]-\tfrac{2}{b}\textstyle\sum_j [p_j] + \tfrac{2a}{b}[p_i])\,.\end{aligned}$$

Equation C.1.1e: The symbol of this is

$$\frac{2b}{a}\left(\left\{\frac{1}{1-p_i}\right\}_4 \otimes \frac{1}{1-p_i} - \left\{\frac{1-x}{1-p_i}\right\}_4 \otimes \frac{1-x}{1-p_i} - \left\{\frac{1-1/x}{1-p_i}\right\}_4 \otimes \frac{1-1/x}{1-p_i}\right)\,.$$

The terms gather as follows, to give

$$\mathcal{S}(\text{Equation C.1.1e}) = \sum_i -\frac{2b}{a}\left(\left\{\tfrac{1}{1-p_i}\right\}_4 - \left\{\tfrac{1-x}{1-p_i}\right\}_4 - \left\{\tfrac{1-1/x}{1-p_i}\right\}_4\right)\otimes$$

$$\begin{aligned}
&\otimes\left(\tfrac{1}{b}\textstyle\sum_j[p_j]-\tfrac{a}{b}[p_i]\right)+\\
&-\frac{2b}{a}\left(\left\{\tfrac{1-x}{1-p_i}\right\}_4+\left\{\tfrac{1-1/x}{1-p_i}\right\}_4\right)\otimes(1-x)+\\
&+\frac{2b}{a}\left\{\tfrac{1-1/x}{1-p_i}\right\}_4\otimes x\,.
\end{aligned}$$

Equation C.1.1f: The symbol of this is

$$-\frac{2b}{c}\left(\left\{\frac{1}{1-1/p_i}\right\}_4\otimes\frac{1}{1-1/p_i}-\left\{\frac{1-x}{1-1/p_i}\right\}_4\otimes\frac{1-x}{1-1/p_i}-\left\{\frac{1-1/x}{1-1/p_i}\right\}_4\otimes\frac{1-1/x}{1-1/p_i}\right)\,.$$

The terms gather as follows, to give

$$\begin{aligned}
\mathcal{S}(\text{Equation C.1.1f})=\sum_i\frac{2b}{c}&\left(\left\{\tfrac{1}{1-1/p_i}\right\}_4-\left\{\tfrac{1-x}{1-1/p_i}\right\}_4-\left\{\tfrac{1-1/x}{1-1/p_i}\right\}_4\right)\otimes\\
&\otimes\left(-[p_i]+\tfrac{1}{b}\textstyle\sum_j[p_j]-\tfrac{a}{b}[p_i]\right)+\\
&+\frac{2b}{c}\left(\left\{\tfrac{1-x}{1-1/p_i}\right\}_4+\left\{\tfrac{1-1/x}{1-1/p_i}\right\}_4\right)\otimes(1-x)+\\
&-\frac{2b}{c}\left\{\tfrac{1-1/x}{1-1/p_i}\right\}_4\otimes x\,.
\end{aligned}$$

Now we can gather all of the terms of the symbol of the RHS of Equation C.1.1.

$$\begin{aligned}
&\mathcal{S}(\text{Equation C.1.1 RHS})=\\
&\quad\Big(-c\{x\}_4-2b\{1-1/x\}_4+\\
&\qquad-\frac{2}{bc(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_4-\frac{2}{ab(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_4+\\
&\qquad+(\tfrac{c-a}{2b}+2)\sum_i\{xp_i\}_4+(\tfrac{c-a}{2b}-2)\sum_i\left\{\frac{x}{p_i}\right\}_4+\\
&\qquad+\frac{b}{2(c-a)}\sum_i\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_4+\\
&\qquad+\frac{2b}{a}\sum_i\left\{\tfrac{1-1/x}{1-p_i}\right\}_4-\frac{2b}{c}\sum_i\left\{\tfrac{1-1/x}{1-1/p_i}\right\}_4\Big)\otimes x+\\
&\quad+\Bigg(2b\{1-x\}_4+2b\{1-1/x\}_4+\\
&\qquad-\frac{2}{ac(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_4-\frac{2}{ac(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_4+\\
&\qquad-\sum_j\Bigg(\frac{b}{c-a}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_4+\\
&\quad-\frac{2b}{a}\left\{\tfrac{1-x}{1-p_i}\right\}_4-\frac{2b}{a}\left\{\tfrac{1-1/x}{1-p_i}\right\}_4+\frac{2b}{c}\left\{\tfrac{1-x}{1-1/p_i}\right\}_4+\frac{2b}{c}\left\{\tfrac{1-1/x}{1-1/p_i}\right\}_4\Bigg)\Bigg)\otimes(1-x)+\\
&\quad+\sum_i\Bigg(\frac{2}{abc(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_4+\frac{2}{abc(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_4+\\
&\qquad+(\tfrac{c-a}{2b}+2)\{xp_i\}_4-(\tfrac{c-a}{2b}-2)\left\{\frac{x}{p_i}\right\}_4+
\end{aligned}\tag{C.2.1}$$

$$+\sum_j \left(\frac{1}{c-a} \left\{ \frac{(1-x)^2}{x} \frac{p_j}{(1-p_j)^2} \right\}_4 \right) + \frac{1}{2} \left\{ \frac{(1-x)^2}{x} \frac{p_i}{(1-p_i)^2} \right\}_4 +$$
$$-\frac{2}{a} \sum_j \left(\left\{ \tfrac{1}{1-p_j} \right\}_4 - \left\{ \tfrac{1-x}{1-p_j} \right\}_4 - \left\{ \tfrac{1-1/x}{1-p_j} \right\}_4 \right) - 2 \left(\left\{ \tfrac{1}{1-p_i} \right\}_4 - \left\{ \tfrac{1-x}{1-p_i} \right\}_4 - \left\{ \tfrac{1-1/x}{1-p_i} \right\}_4 \right) +$$
$$+\frac{2}{c} \sum_j \left(\left\{ \tfrac{1}{1-1/p_j} \right\}_4 - \left\{ \tfrac{1-x}{1-1/p_j} \right\}_4 - \left\{ \tfrac{1-1/x}{1-1/p_j} \right\}_4 \right) +$$
$$+ 2 \left(\left\{ \tfrac{1}{1-1/p_i} \right\}_4 - \left\{ \tfrac{1-x}{1-1/p_i} \right\}_4 - \left\{ \tfrac{1-1/x}{1-1/p_i} \right\}_4 \right) \Bigg) \otimes p_i \,.$$

C.2.2 Symbol of the left hand side

For the LHS we need a good way of writing the symbol of $I_{4,1}(x,y)$, modulo $\sqcup\!\sqcup$. Or at least a good way of writing the symbol of $I^-_{4,1}(x,y)$, modulo $\sqcup\!\sqcup$.

Perhaps the nicest expression for the symbol of $I_{4,1}(x,y)$ mod $\sqcup\!\sqcup$ is the one given in Proposition 7.4.3, which gives it a structure similar to that of κ, and the 'ϕ_5' element Goncharov defines. Recall that this states

Proposition 7.4.3. *Modulo products, the symbol of $I_{4,1}(x,y)$ be can be expressed as follows.*

$$\begin{aligned} I_{4,1}(x,y) &\overset{\sqcup\!\sqcup}{=} \\ &- 3 \left\{ \frac{x}{y} \right\}_5 - \{x\}_5 - \{y\}_5 + \\ &+ \left\{ \frac{x}{y} \right\}_4 \otimes \frac{1-x}{1-y} + \{x\}_4 \otimes (1-y) + \{y\}_4 \otimes (1-x) + \\ &- \left(\{1-x\}_3 + \{1-y\}_3 - \left\{ \frac{1-x}{1-y} \right\}_3 + \left\{ \frac{1-1/x}{1-1/y} \right\}_3 \right) \otimes \frac{x}{y} \otimes \frac{x}{y} + \\ &+ \left(\{x\}_3 \otimes (1-y) - \{y\}_3 \otimes (1-x) + \left\{ \frac{x}{y} \right\}_3 \otimes \frac{1-x}{1-y} \right) \otimes \frac{x}{y} \,, \end{aligned}$$

where we write $\{x\}_n$ to mean $-(1-x) \wedge x \otimes x^{n-2}$.

We therefore obtain the following expression for the symbol of $I^-_{4,1}(x,y)$, by summing $I_{4,1}(x,y)$ and $-I_{4,1}(x,\frac{1}{y})$. There are a few simplifications to make immediately using $\left\{ \frac{1}{y} \right\}_n = -(-1)^n \{y\}_n$.

$$\begin{aligned} I_{4,1}(x,y) - I_{4,1}(x,\frac{1}{y}) &\overset{\sqcup\!\sqcup}{=} \\ &- 3 \left\{ \frac{x}{y} \right\}_5 + 3 \{xy\}_5 \quad + 2 \{y\}_4 \otimes (1-x) + \\ &+ \left\{ \frac{x}{y} \right\}_4 \otimes \frac{1-x}{1-y} + \{x\}_4 \otimes (1-y) - \{xy\}_4 \otimes \frac{1-x}{1-1/y} - \{x\}_4 \otimes (1-1/y) + \\ &- \left(\{1-x\}_3 + \{1-y\}_3 - \left\{ \frac{1-x}{1-y} \right\}_3 + \left\{ \frac{1-1/x}{1-1/y} \right\}_3 \right) \otimes \frac{x}{y} \otimes \frac{x}{y} + \\ &+ \left(\{1-x\}_3 + \{1-1/y\}_3 - \left\{ \frac{1-x}{1-1/y} \right\}_3 + \left\{ \frac{1-1/x}{1-y} \right\}_3 \right) \otimes xy \otimes xy + \\ &+ \left(\{x\}_3 \otimes (1-y) - \{y\}_3 \otimes (1-x) + \left\{ \frac{x}{y} \right\}_3 \otimes \frac{1-x}{1-y} \right) \otimes \frac{x}{y} \end{aligned}$$

$$-\left(\{x\}_3 \otimes (1-1/y) - \{1/y\}_3 \otimes (1-x) + \{xy\}_3 \otimes \frac{1-x}{1-1/y}\right) \otimes xy\,,$$

Now sum over $y = p_i$, to obtain the LHS of the identity in Equation C.1.1. We obtain

$$\begin{aligned}
&I_{4,1}(x, \sum_i [p_i]) - I_{4,1}(x, \sum_i [\tfrac{1}{p_i}]) \overset{\sqcup\!\sqcup}{=} \\
&\sum_i \Big(-3\left\{\frac{x}{p_i}\right\}_4 \otimes \frac{x}{p_i} + 3\{xp_i\}_4 \otimes (xp_i) \quad + 2\{p_i\}_4 \otimes (1-x) + \\
&\quad + \left\{\frac{x}{p_i}\right\}_4 \otimes \frac{1-x}{1-p_i} + \{x\}_4 \otimes (1-p_i) - \{xp_i\}_4 \otimes \frac{1-x}{1-1/p_i} - \{x\}_4 \otimes (1-1/p_i) + \\
&\quad - \left(\{1-x\}_3 + \{1-p_i\}_3 - \left\{\frac{1-x}{1-p_i}\right\}_3 + \left\{\frac{1-1/x}{1-1/p_i}\right\}_3\right) \otimes \frac{x}{p_i} \otimes \frac{x}{p_i} + \\
&\quad + \left(\{1-x\}_3 + \{1-1/p_i\}_3 - \left\{\frac{1-x}{1-1/p_i}\right\}_3 + \left\{\frac{1-1/x}{1-p_i}\right\}_3\right) \otimes xp_i \otimes xp_i + \\
&\quad + \left(\{x\}_3 \otimes (1-p_i) - \{p_i\}_3 \otimes (1-x) + \left\{\frac{x}{p_i}\right\}_3 \otimes \frac{1-x}{1-p_i}\right) \otimes \frac{x}{p_i} + \\
&\quad - \left(\{x\}_3 \otimes (1-1/p_i) - \{1/p_i\}_3 \otimes (1-x) + \{xp_i\}_3 \otimes \frac{1-x}{1-1/p_i}\right) \otimes xp_i\Big)\,.
\end{aligned}$$

Gather by the last tensor factor to obtain

$$\begin{aligned}
&\mathcal{S}(\text{Equation C.1.1 LHS}) \overset{\sqcup\!\sqcup}{=} \\
&\sum_j \Bigg(-3\left\{\frac{x}{p_j}\right\}_4 + 3\{xp_j\}_4 + \\
&\quad - \left(\{1-x\}_3 + \{1-p_j\}_3 - \left\{\frac{1-x}{1-p_j}\right\}_3 + \left\{\frac{1-1/x}{1-1/p_j}\right\}_3\right) \otimes \frac{x}{p_j} + \\
&\quad + \left(\{1-x\}_3 + \{1-1/p_j\}_3 - \left\{\frac{1-x}{1-1/p_j}\right\}_3 + \left\{\frac{1-1/x}{1-p_j}\right\}_3\right) \otimes xp_j + \\
&\quad + \left(\{x\}_3 \otimes (1-p_j) - \{p_j\}_3 \otimes (1-x) + \left\{\frac{x}{p_j}\right\}_3 \otimes \frac{1-x}{1-p_j}\right) + \\
&\quad - \left(\{x\}_3 \otimes (1-1/p_j) - \{1/p_j\}_3 \otimes (1-x) + \{xp_j\}_3 \otimes \frac{1-x}{1-1/p_j}\right)\Bigg) \otimes x + \\
&+ \left(\sum_j \left\{\frac{x}{p_j}\right\}_4 - \sum_j \{xp_j\}_4 + 2\sum_j \{p_i\}_4\right) \otimes (1-x) + \qquad \text{(C.2.2)} \\
&+ \sum_i \Bigg(3\left\{\frac{x}{p_i}\right\}_4 + 3\{xp_i\}_4 \quad - \{xp_i\}_4 + \{x\}_4 + \\
&\quad + \frac{a}{b}\left(\left\{\frac{x}{p_i}\right\}_4 - \{xp_i\}_4\right) - \frac{1}{b}\sum_j \left(\left\{\frac{x}{p_j}\right\}_4 - \{xp_j\}_4\right) + \\
&\quad + \left(\{1-x\}_3 + \{1-p_i\}_3 - \left\{\frac{1-x}{1-p_i}\right\}_3 + \left\{\frac{1-1/x}{1-1/p_i}\right\}_3\right) \otimes \frac{x}{p_i} +
\end{aligned}$$

$$+\left(\{1-x\}_3+\{1-1/p_i\}_3-\left\{\frac{1-x}{1-1/p_i}\right\}_3+\left\{\frac{1-1/x}{1-p_i}\right\}_3\right)\otimes xp_i+$$
$$-\left(\{x\}_3\otimes(1-p_i)-\{p_i\}_3\otimes(1-x)+\left\{\frac{x}{p_i}\right\}_3\otimes\frac{1-x}{1-p_i}\right)+$$
$$-\left(\{x\}_3\otimes(1-1/p_i)-\{1/p_i\}_3\otimes(1-x)+\{xp_i\}_3\otimes\frac{1-x}{1-1/p_i}\right)\Bigg)\otimes p_i\,.$$

C.2.3 Comparing both sides

Now we begin to compare both sides to show they are equal. We look at the difference between Equation C.2.2 and Equation C.2.1. To do this, we first need the following result.

Proposition C.2.2. *The following combination is a functional equation for* Li_4*:*

$$\begin{aligned}\mathcal{F}:=&-2b\,\{1-x\}_4-2b\,\{1-1/x\}_4+\\&+\frac{2}{ac(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_4+\frac{2}{ac(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_4+\\&+\sum_i\Bigg(\frac{b}{c-a}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_4+\\&\quad+\frac{2b}{a}\left\{\tfrac{1-x}{1-p_i}\right\}_4+\frac{2b}{a}\left\{\tfrac{1-1/x}{1-p_i}\right\}_4+\\&\quad-\frac{2b}{c}\left\{\tfrac{1-x}{1-1/p_i}\right\}_4-\frac{2b}{c}\left\{\tfrac{1-1/x}{1-1/p_i}\right\}_4+\\&\quad+\left\{\frac{x}{p_i}\right\}_4-\{xp_i\}_4+2\,\{p_i\}_4\Bigg)=0\,.\end{aligned}$$

Proof. This arises by expanding out the κ element (essentially $I_{3,1}$) applied to the two term relation $\{x\}_2+\left\{\frac{1}{x}\right\}_2$, and the algebraic Li_2 equation $\sum_i\{p_i\}_2$, in two different ways. These expansions are given in [Gan00], where the expression for $\kappa([x]+[\frac{1}{x}],y)$ comes originaly from Zagier.

The difference between the two expansions of

$$\kappa\left([x]+[\tfrac{1}{x}],\sum_i[p_i]\right)$$

vanishes modulo $ш$. Scaling the result by $\frac{-2b}{c-a}$, and adding $\frac{4bc}{c-a}$ times the algebraic Li_4 equation produces the combination $\mathcal{F}$. Some simplifications using $\#\text{roots}=-c$ are necessary. □

C.2.3.1 Factors ending $\otimes(1-x)$

Let us compare the $\otimes(1-x)$ factor of both sides, to see if they are equal. We see that the difference is the combination $\mathcal{F}$, from Proposition C.2.2 so the two sides are equal.

C.2.3.2 Factors ending $\otimes p_i$

Now consider the $\otimes p_i$ factor of both sides. Take the difference of the LHS − RHS, then we can can add $\frac{1}{b}\mathcal{F}$ to obtain, after some simplification

$$\begin{aligned}
\Bigg(& 2\left\{1-x\right\}_4 + 2\left\{1-1/x\right\}_4 - \left\{x\right\}_4 + \\
& -\frac{1}{2}\left\{xp_i\right\}_4 - \frac{1}{2}\left\{\frac{x}{p_i}\right\}_4 + \\
& +\frac{1}{2}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_4 - \frac{2}{b}\sum_j \left\{p_j\right\}_4 + \\
& -\frac{2}{a}\sum_j \left(\left\{\tfrac{1}{1-p_j}\right\}_4\right) + 2\left(\left\{\tfrac{1}{1-p_i}\right\}_4 - \left\{\tfrac{1-x}{1-p_i}\right\}_4 - \left\{\tfrac{1-1/x}{1-p_i}\right\}_4\right) + \\
& +\frac{2}{c}\sum_j \left(\left\{\tfrac{1}{1-1/p_j}\right\}_4\right) + 2\left(\left\{\tfrac{1}{1-1/p_i}\right\}_4 - \left\{\tfrac{1-x}{1-1/p_i}\right\}_4 - \left\{\tfrac{1-1/x}{1-1/p_i}\right\}_4\right) + \\
& -\left(\left\{1-x\right\}_3 + \left\{1-p_i\right\}_3 - \left\{\frac{1-x}{1-p_i}\right\}_3 + \left\{\frac{1-1/x}{1-1/p_i}\right\}_3\right) \otimes \frac{x}{p_i} + \\
& -\left(\left\{1-x\right\}_3 + \left\{1-1/p_i\right\}_3 - \left\{\frac{1-x}{1-1/p_i}\right\}_3 + \left\{\frac{1-1/x}{1-p_i}\right\}_3\right) \otimes xp_i + \\
& +\left(\left\{x\right\}_3 \otimes (1-p_i) - \left\{p_i\right\}_3 \otimes (1-x) + \left\{\frac{x}{p_i}\right\}_3 \otimes \frac{1-x}{1-p_i}\right) + \\
& +\left(\left\{x\right\}_3 \otimes (1-1/p_i) - \left\{1/p_i\right\}_3 \otimes (1-x) + \left\{xp_i\right\}_3 \otimes \frac{1-x}{1-1/p_i}\right)\Bigg) \otimes p_i \,.
\end{aligned} \tag{C.2.3}$$

Now recall the algebraic Li_4 functional equation from Proposition 7.3.7. It says that

Proposition 7.3.7 (Algebraic Li_4 equation, Lemma 4.1, Equation (4.1.6), in [Gan95])**.** *The following is a functional equation for* Li_4.

$$\mathrm{Li}_4\left(\sum_i \frac{1}{a}\left[\frac{1}{1-p_i}\right] + \frac{1}{b}\left[p_i\right] + \frac{1}{c}\left[1-\frac{1}{p_i}\right]\right) \overset{\sqcup\!\sqcup}{=} 0\,,$$

where c is defined by $a+b+c=0$.

Multiplying the functional equation in this result by 2, and inverting the last argument shows that

$$\frac{2}{a}\sum_j \left(\left\{\tfrac{1}{1-p_j}\right\}_4\right) + \frac{2}{b}\sum_j \left\{p_j\right\}_4 - \frac{2}{c}\sum_j \left(\left\{\tfrac{1}{1-1/p_j}\right\}_4\right) = 0\,.$$

Use this to kill the three sums in Equation C.2.3. Now expand out and gather by the fourth tensor factor of the remainder. Use $\left\{\alpha\right\}_4 = \left\{\alpha\right\}_3 \otimes \alpha$, and don't bother converting $1-p_i$ into p_j's. We obtain the following

$$\begin{aligned}
\Bigg(& 2\left\{x\right\}_3 + 2\left\{1-1/x\right\}_3 + \left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_3 + \\
& -2\left\{\frac{1-x}{1-p_i}\right\}_3 - 2\left\{\frac{1-1/x}{1-p_i}\right\}_3 - 2\left\{\frac{1-x}{1-1/p_i}\right\}_3 - 2\left\{\frac{1-1/x}{1-1/p_i}\right\}_3 + \\
& -2\left\{p_i\right\}_3 + \left\{\frac{x}{p_i}\right\}_3 + \left\{xp_i\right\}_3\Bigg) \otimes (1-x) \otimes p_i +
\end{aligned}$$

$$
\begin{aligned}
&+ \Bigg(-2\{1-1/x\}_3 - \{x\}_3 - \frac{1}{2}\{xp_i\}_3 - \frac{1}{2}\left\{\frac{x}{p_i}\right\}_3 + \\
&\quad -\frac{1}{2}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_3 + \left\{\frac{1-1/x}{1-p_i}\right\}_3 + \left\{\frac{1-1/x}{1-1/p_i}\right\}_3 + \\
&\quad -\{1-1/p_i\}_3 + \left\{\frac{1-x}{1-p_i}\right\}_3 + \left\{\frac{1-x}{1-1/p_i}\right\}_3 \Bigg) \otimes x \otimes p_i + \\
&+ \Bigg(\frac{1}{2}\{xp_i\}_3 + \frac{1}{2}\left\{\frac{x}{p_i}\right\}_3 + \frac{1}{2}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i}{}^2)\right\}_3 + \\
&\quad +\{1-1/p_i\}_3 - \left\{\frac{1-x}{1-1/p_i}\right\}_3 - \left\{\frac{1-1/x}{1-1/p_i}\right\}_3 + \\
&\quad +\{1-p_i\}_3 - \left\{\frac{1-x}{1-p_i}\right\}_3 - \left\{\frac{1-1/x}{1-p_i}\right\}_3 - \{x\}_3 \Bigg) \otimes p_i \otimes p_i + \\
&+ \Bigg(-\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_3 - 2\{1-p_i\}_3 + 2\left\{\frac{1-x}{1-p_i}\right\}_3 + 2\left\{\frac{1-1/x}{1-p_i}\right\}_3 + \\
&\quad -2\{1-1/p_i\}_3 + 2\left\{\frac{1-x}{1-1/p_i}\right\}_3 + 2\left\{\frac{1-1/x}{1-1/p_i}\right\}_3 + \\
&\quad +2\{x\}_3 - \left\{\frac{x}{p_i}\right\}_3 - \{xp_i\}_3 \Bigg) \otimes (1-p_i) \otimes p_i \,.
\end{aligned}
\tag{C.2.4}
$$

Recall the 3-term identity for Li_3. Also recall Kummer's functional equation for Li_3.

Lemma C.2.3 (3-term)**.** *The following combination is a functional equation for* Li_3

$$\mathcal{T} \coloneqq \{x\}_3 + \{1-x\}_3 + \{1-1/x\}_3 = 0\,.$$

Proposition C.2.4 (Kummer)**.** *The following combination is a functional equation for* Li_3

$$
\begin{aligned}
\mathcal{K}_{x,y} \coloneqq & -\left\{\frac{(1-x)^2}{x}\frac{y}{(1-y)^2}\right\}_3 - \left\{\frac{x}{y}\right\}_3 - \{xy\}_3 + 2\{y\}_3 + 2\{x\}_3 + \\
& +2\left\{\frac{1-x}{1-y}\right\}_3 + 2\left\{\frac{1-x}{1-1/y}\right\}_3 + 2\left\{\frac{1-1/x}{1-y}\right\}_3 + 2\left\{\frac{1-1/x}{1-1/y}\right\}_3 = 0\,.
\end{aligned}
$$

We can use these functional equations to show that the expression in Equation C.2.4 vanishes. Specifically it is equal to

$$
\begin{aligned}
&(\mathcal{K}_{x,p_i} - 2\mathcal{T}_x) \otimes (1-x) \otimes p_i + (-\tfrac{1}{2}\mathcal{K}_{x,p_i} + 2\mathcal{T}_x + \mathcal{T}_{p_i}) \otimes x \otimes p_i + \\
&+ (\tfrac{1}{2}\mathcal{K}_{x,p_i} - \mathcal{T}_{p_i}) \otimes p_i \otimes p_i + (-\mathcal{K}_{x,p_i} + 2\mathcal{T}_{p_i}) \otimes (1-p_i) \otimes p_i = 0\,.
\end{aligned}
$$

So the difference between the $\otimes p_i$ factors is zero, meaning the factors on both sides are equal.

C.2.3.3 Factors ending $\otimes x$

Now consider the $\otimes x$ factor. Expand out, and gather by the fourth factor. This time, convert the $1-p_i$ terms to p_j's when gathering. We obtain

$$\Bigg(-c\{x\}_3 + 2b\{1-1/x\}_3 +$$

$$
\begin{aligned}
&+\frac{2a}{bc(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_3+\frac{2c}{ab(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_3+\\
&+\sum_j\Bigg(\left(\frac{c-a}{2b}-1\right)\{xp_j\}_3+\left(\frac{c-a}{2b}-1\right)\left\{\frac{x}{p_j}\right\}_3-\frac{b}{2(c-a)}\left\{\frac{(1-x)^2}{x}\frac{p_j}{(1-p_j)^2}\right\}_3+\\
&\quad-\frac{2b}{a}\left\{\frac{1-1/x}{1-p_j}\right\}_3+\frac{2b}{c}\left\{\frac{1-1/x}{1-1/p_j}\right\}_3+\{1-p_j\}_3-\{1-1/p_j\}_3+\\
&\quad-\left\{\frac{1-x}{1-p_j}\right\}_3+\left\{\frac{1-1/x}{1-1/p_j}\right\}_3+\left\{\frac{1-x}{1-1/p_j}\right\}_3-\left\{\frac{1-1/x}{1-p_j}\right\}_3\Bigg)\Bigg)\otimes x\otimes x+\\
+&\Bigg(-2b\{1-1/x\}_3+\\
&+\frac{2}{c(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_3+\frac{2}{a(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_3+\\
&+\sum_j\Bigg(\frac{b}{c-a}\left\{\frac{(1-x)^2}{x}\frac{p_j}{(1-p_j)^2}\right\}_3+\frac{2b}{a}\left\{\frac{1-1/x}{1-p_j}\right\}_3+\\
&\quad-\frac{2b}{c}\left\{\frac{1-1/x}{1-1/p_j}\right\}_3-\left\{\frac{x}{p_j}\right\}_3+\{xp_j\}_3\Bigg)\Bigg)\otimes(1-x)\otimes x+
\end{aligned}
\tag{C.2.5}
$$

$$
\begin{aligned}
+&\sum_i\Bigg(\frac{-2}{bc(c-a)}\left\{\frac{t}{x^a(1-x)^b}\right\}_3+\frac{-2}{ab(c-a)}\left\{\frac{t}{x^c(x-1)^b}\right\}_3+\\
&\quad+\left(\frac{c-a}{2b}-1\right)\{xp_i\}_3-\left(\frac{c-a}{2b}+1\right)\left\{\frac{x}{p_i}\right\}_3+\\
&+\frac{b}{2(c-a)}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_3-\frac{2b}{c}\left\{\frac{1-1/x}{1-1/p_i}\right\}_3-2\{1-x\}_3+\\
&-\{1-p_i\}_3+\left\{\frac{1-x}{1-p_i}\right\}_3-\left\{\frac{1-1/x}{1-1/p_i}\right\}_3-\{1-1/p_i\}_3+\\
&+\left\{\frac{1-x}{1-1/p_i}\right\}_3-\left\{\frac{1-1/x}{1-p_i}\right\}_3-\{x\}_3+\{xp_i\}_3+\\
&+\frac{1}{b}\sum_j\Bigg(\frac{-b}{c-a}\left\{\frac{(1-x)^2}{x}\frac{p_j}{(1-p_j)^2}\right\}_3-\frac{2b}{a}\left\{\frac{1-1/x}{1-p_j}\right\}_3+\\
&\quad+\frac{2b}{c}\left\{\frac{1-1/x}{1-1/p_j}\right\}_3+\left\{\frac{x}{p_j}\right\}_3-\{xp_j\}_3\Bigg)+\\
&-\frac{a}{b}\Bigg(\frac{-b}{c-a}\left\{\frac{(1-x)^2}{x}\frac{p_i}{(1-p_i)^2}\right\}_3-\frac{2b}{a}\left\{\frac{1-1/x}{1-p_i}\right\}_3+\\
&\quad+\frac{2b}{c}\left\{\frac{1-1/x}{1-1/p_i}\right\}_3+\left\{\frac{x}{p_i}\right\}_3-\{xp_i\}_3\Bigg)\Bigg)\otimes p_i\otimes x\,.
\end{aligned}
$$

Recall from Gangl [Gan00], the following Li_3 functional equation, and also a related version

Proposition C.2.5. *The following are functional equations for* Li_3

$$
\mathcal{G}_1:=\frac{1}{abc}\left\{\frac{t}{x^a(1-x)^b}\right\}_3+\sum_j\left(\frac{1}{a}\left\{\frac{1-x}{1-p_j}\right\}_3+\frac{1}{c}\left\{\frac{1-1/x}{1-1/p_j}\right\}_3+\right.
$$

$$+\frac{1}{b}\left\{\frac{x}{p_j}\right\}_3 - \frac{1}{a}\{1-p_j\}_3\Bigg) + \{1-1/x\}_3 = 0$$

$$\mathcal{G}_2 := \frac{1}{abc}\left\{\frac{t}{x^c(x-1)^b}\right\}_3 + \sum_j \Bigg(\frac{1}{c}\left\{\frac{1-x}{1-1/p_j}\right\}_3 + \frac{1}{a}\left\{\frac{1-1/x}{1-p_j}\right\}_3 +$$
$$+\frac{1}{b}\{xp_j\}_3 - \frac{1}{c}\{1-1/p_j\}_3\Bigg) + \{1-x\}_3 = 0\,.$$

Proof. One equation comes directly from Gangl [Gan00]. The other can be obtained by setting $x \mapsto 1/x$, and using that

$$\sum_j \frac{1}{a}\{1-p_j\}_3 = \sum_j \frac{1}{c}\{1-1/p_j\}_3\,.$$

This can be obtained by by writing $\{p_j\}_3 = -\{1-1/p_j\}_3 - \{1-p_j\}_3$ using the 3-term relation, and substituting this into the algebraic Li_3 equation

$$\sum_j -\frac{1}{a}\{1-p_j\}_3 + \frac{1}{b}\{p_j\}_3 = 0\,,$$

given in Proposition 7.3.5 □

If we use these, and the equations in previous propositions, we see that all factors here cancel, as follows. The expression in Equation C.2.5 is equal to

$$\frac{1}{c-a}\Bigg(2a^2\mathcal{G}_1 + 2c^2\mathcal{G}_2 + \frac{b}{2}\sum_j \mathcal{K}_{x,p_j} - b\sum_j \mathcal{T}_{p_j} - 2c^2\mathcal{T}_x\Bigg) \otimes x \otimes x +$$
$$+\frac{1}{c-a}\Bigg(2ab\mathcal{G}_1 + 2bc\mathcal{G}_2 - b\sum_j \mathcal{K}_{x,p_j} + 2b\sum_j \mathcal{T}_{p_j} - 2bc\mathcal{T}_x\Bigg) \otimes (1-x) \otimes x +$$
$$+\frac{1}{c-a}\sum_i \Bigg(-2a\mathcal{G}_1 - 2c\mathcal{G}_2 + \sum_j \mathcal{K}_{x,p_j} - 2\sum_j \mathcal{T}_{p_j} +$$
$$+\frac{c-a}{2}\mathcal{K}_{x,p_i} + (c-a)\mathcal{T}_{p_i} - 2a\mathcal{T}_x\Bigg) \otimes p_i \otimes x = 0\,.$$

This shows that the difference of the $\otimes x$ factors of the two sides is 0, so they are equal.

C.2.4 End of proof

The results in the above subsections show that both sides agree exactly. Section C.2.3.1 shows that the $\otimes(1-x)$ factors agree, Section C.2.3.2 shows that the $\otimes p_i$ factors agree, and Section C.2.3.3 shows that the $\otimes x$ factors agree on both sides. Combining these subsections completes the proof of the identity in Theorem C.1.1. □