Special Values of Multidimensional Polylogarithms

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Abstract. Historically, the polylogarithm has attracted specialists and non-specialists alike with its lovely evaluations. Much the same can be said for Euler sums (or multiple harmonic sums), which, within the past decade, have arisen in combinatorics, knot

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theory and high-energy physics. More recently, we have been forced to consider multidimensional extensions encompassing the classical polylogarithm, Euler sums, and the Riemann zeta function. Here, we provide a general framework within which previously isolated results can now be properly understood. Applying the theory developed herein, we prove several previously conjectured evaluations, including a longstanding conjecture of Don Zagier.

1 Introduction

We are going to study a class of multiply nested sums of the form

$$\lambda\binom{s_1,\ldots,s_k}{b_1,\ldots,b_k} := \prod_{j=1}^{k}\sum_{\nu_j=1}^{\infty} b_j^{-\nu_j}\left(\sum_{i=j}^{k}\nu_i\right)^{-s_j}, \tag{1}$$

and which we shall refer to as *multidimensional polylogarithms.* When $k=0$, the usual convention on empty products gives $\lambda(\{\}) := 1$, where $\{\}$ denotes the empty string. When $k=1$, note that

$$\lambda\binom{s}{b} = \sum_{\nu=1}^{\infty}\frac{1}{\nu^s b^\nu} = \mathrm{Li}_s\left(\frac{1}{b}\right) \tag{2}$$

is the usual polylogarithm [36, 37] when s is a positive integer and $|b|\ge 1$. Of course, the polylogarithm (2) reduces to the classical Riemann zeta function [19, 31, 43]

$$\zeta(s) = \sum_{\nu=1}^{\infty}\frac{1}{\nu^s}, \quad \Re(s)>1, \tag{3}$$

when $b=1$. More generally, for any $k>0$ write

$$n_j = \sum_{i=j}^{k}\nu_i \quad \text{and} \quad b_j = \prod_{i=1}^{j} a_i, \quad j=1,2,\ldots,k.$$

Then

$$\lambda\binom{s_1,\ldots,s_k}{b_1,\ldots,b_k} = \sum_{n_1>\cdots>n_k>0}\prod_{j=1}^{k} n_j^{-s_j}a_j^{-n_j}. \tag{4}$$

These latter sums, with each $a_j = 1$ (sometimes called *"Euler sums"*), have been studied previously at various levels of generality [2, 4, 5, 7, 9, 11, 12, 13, 24, 28, 29, 30, 38, 39], the case $k=2$ going back to Euler [20]. Recently, such sums have arisen in combinatorics (analysis of quad-trees [23, 34] and of lattice reduction algorithms [16]), knot theory [11, 12, 13, 35], and high-energy particle physics [9] (quantum field theory).

In view of these recent applications and the well-known fact that the polylogarithm (2) often arises in physical problems via the multiple integration of rational forms, one might expect that the more general multidimensional polylogarithm (1) would likewise find application in a wide variety of physical contexts. Nevertheless, lest it be suspected that the authors have embarked on a program of generalization for its own sake, let the reader be assured that it was only with the greatest reluctance that we arrived at the definition (1). On the one hand, the polylogarithm (2) has traditionally been studied as a function of b with the positive integer s fixed; while on the other hand, the Riemann zeta function (3) and its nested-sum generalization (4) have typically been studied as functions of the s_j, with the a_j and b_j specialized to ± 1. However, we have found, in the course of our investigations, that a great deal of insight is lost by ignoring the interplay between these related sums when both sequences of parameters s_j and b_j are permitted to vary. Indeed, it is our view that it is *impossible* to fully understand the sums (2–4) without viewing them as members of a broader class of multidimensional polylogarithms (1).

Don Zagier (see eg. [44]) has argued persuasively in favour of studying special values of zeta functions at integer arguments, as these values "often seem to dictate the most important properties of the objects to which the zeta functions are associated." It seems appropriate, therefore, to focus on the values the multidimensional polylogarithms (1) take when the s_j are restricted to the set of positive integers, despite the fact that the sums (1) and their special cases have a rich structure as analytic functions of the complex variables s_j. However, we allow the parameters b_j to take on complex values, with each $|b_j| \ge 1$ and $(b_1, s_1) \ne (1,1)$ to ensure convergence.

Their importance notwithstanding, we feel obliged to confess that our interest in special values extends beyond mere utilitarian concerns. Lewin [36] (p. xi) writes of a "school-boy fascination" with certain numerical results, an attitude which we wholeheartedly share. In the hope that the reader might also be convinced of the intrinsic beauty of the subject, we offer two modest examples. The first [28, 35],

$$\prod_{j=1}^{k} \sum_{\nu_j=1}^{\infty} \frac{1}{(\nu_j + \cdots + \nu_k)^2} = \frac{\pi^{2k}}{(2k+1)!}, \quad k \ge 0,$$

generalizes Euler's celebrated result

$$\zeta(2) = \sum_{\nu=1}^{\infty} \frac{1}{\nu^2} = \frac{\pi^2}{6},$$

and is extended to all even positive integer arguments in [5]. The second (see Corollary 1 of Section 8),

$$\prod_{j=1}^{k} \sum_{\nu_j=1}^{\infty} \frac{(-1)^{\nu_j+1}}{\nu_j + \cdots + \nu_k} = \prod_{j=1}^{k} \sum_{\nu_j=1}^{\infty} \frac{1}{2^{\nu_j}(\nu_j + \cdots + \nu_k)} = \frac{(\log 2)^k}{k!}, \quad k \ge 0 \tag{5}$$

can be viewed as a multidimensional extension of the elementary "dual" Maclaurin series evaluations

$$\sum_{\nu=1}^{\infty} \frac{(-1)^{\nu+1}}{\nu} = \sum_{\nu=1}^{\infty} \frac{1}{\nu 2^{\nu}} = \log 2,$$

and leads to deeper questions of duality (Section 6) and computational issues related to series acceleration (Section 7). We state additional results in the next section and outline connections to combinatorics and q-series. In Section 4, we develop several different integral representations, which are then used in subsequent sections to classify various types of identities that multidimensional polylogarithms satisfy. Sections 8 through 12 conclude the paper with proofs of previously conjectured evaluations, including a longstanding conjecture of Zagier [44] and its generalization.

2 Definitions and Additional Examples

A useful specialization of the general multidimensional polylogarithm (1), which is at the same time an extension of the polylogarithm (2), is the case in which each $b_j = b$. Under these circumstances, we write

$$\lambda_b(s_1, \dots, s_k) := \lambda\binom{s_1, \dots, s_k}{b, \dots, b} = \prod_{j=1}^{k} \sum_{\nu_j=1}^{\infty} b^{-\nu_j} \left(\sum_{i=j}^{k} \nu_i\right)^{-s_j}, \tag{6}$$

and distinguish the cases $b = 1$ and $b = 2$ with special symbols:

$$\zeta := \lambda_1 \quad \text{and} \quad \delta := \lambda_2. \tag{7}$$

The latter δ-function represents an iterated sum extension of the polylogarithm (2) with argument one-half, and will play a crucial role in computational issues (Section 7) and "duality" identities such as (5). The former coincides with (4) when $k > 0$ and each $a_j = 1$, and hence can be viewed as a multidimensional unsigned Euler sum. We will follow Zagier [44] in referring to these as *"multiple zeta values"* or *MZVs* for short. By specifying each $b_j = \pm 1$ in (1), *alternating Euler sums* [5] are recovered, and in this case, it is convenient to combine the strings of exponents and signs into a single string with s_j in the jth position when $b_j = +1$, and s_j- in the jth position when $b_j = -1$. To avoid confusion, it should be also noted that in [5] the alternating Euler sums were studied using the notation

$$\zeta(s_1, \dots, s_k) := \sum_{n_1 > n_2 > \dots > n_k} \prod_{j=1}^{k} n_j^{-|s_j|} \sigma_j^{-n_j}$$

where $s_1, \dots, s_k$ are non-zero integers and $\sigma_j := \operatorname{signum}(s_j)$.

Additionally, n repetitions of a substring U will be denoted by U^n. Thus, for example,

$$\lambda(\{2-,1\}^n) := \lambda\begin{pmatrix} 2,1,\ldots,2,1 \\ -1,1,\ldots,-1,1 \end{pmatrix} = \prod_{j=1}^{n} \sum_{\nu_{2j-1}=1}^{\infty} \sum_{\nu_{2j}=1}^{\infty} \frac{(-1)^{\nu_{2j-1}}}{\left(\sum_{i=2j-1}^{k} \nu_i\right)^2 \left(\sum_{i=2j}^{k} \nu_i\right)}.$$

Unit Euler sums, that is those sums (1) in which each $s_j = 1$, are also important enough to be given a distinctive notation. Accordingly, we define

$$\mu(b_1,\ldots,b_k) := \lambda\begin{pmatrix} 1,\ldots,1 \\ b_1,\ldots,b_k \end{pmatrix} = \prod_{j=1}^{k} \sum_{\nu_j=1}^{\infty} b_j^{-\nu_j} \left(\sum_{i=j}^{k} \nu_i\right)^{-1}. \tag{8}$$

To entice the reader, we offer a small but representative sample of evaluations below.

Example 2.1. Euler showed that

$$\zeta(2,1) = \sum_{n=1}^{\infty} \frac{1}{n^2} \sum_{k=1}^{n-1} \frac{1}{k} = \sum_{n=1}^{\infty} \frac{1}{n^3} = \zeta(3),$$

and more generally [20, 39], that

$$2\zeta(m,1) = m\zeta(m+1) - \sum_{k=1}^{m-2} \zeta(m-k)\zeta(k+1), \quad m = 2,3,4,\ldots.$$

The continued interest in Euler sums is evidenced by the fact that a recent American Mathematical Monthly problem [21] effectively asks for the proof of $\zeta(2,1) = \zeta(3)$.

Examples of arbitrary depth evaluations for all nonnegative integers n are provided by

Example 2.2.

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

previously conjectured by Don Zagier [44] and proved herein (see Section 12); and

Example 2.3.

$$\zeta(2,\{1,3\}^n) \stackrel{?}{=} 4^{-n} \sum_{k=0}^{n} (-1)^k \zeta(\{4\}^{n-k}) \left\{ (4k+1)\zeta(4k+2) - 4\sum_{j=1}^{k} \zeta(4j-1)\zeta(4k-4j+3) \right\},$$

conjectured in [5], and which remains unproved.

Example 2.4. An intriguing evaluation involving alternations, conjectured in [5] and proved herein (see Section 8), is

$$\begin{aligned} \mu(\{-1\}^m, 1, \{-1\}^n) &= (-1)^{m+1} \sum_{k=0}^{m} \binom{n+k}{n} A_{k+n+1} P_{m-k} \\ &+ (-1)^{n+1} \sum_{k=0}^{n} \binom{m+k}{m} Z_{k+m+1} P_{n-k}, \end{aligned} \tag{9}$$

where

$$A_r := \mathrm{Li}_r(\tfrac{1}{2}) = \delta(r) = \sum_{k=1}^{\infty} \frac{1}{2^k k^r}, \quad P_r := \frac{(\log 2)^r}{r!}, \quad Z_r := (-1)^r \zeta(r).$$

The formula (9) is valid for all nonnegative integers m and n if the divergent $m = 0$ case is interpreted appropriately.

EXAMPLE 2.5. If the s_j are all nonpositive integers, then

$$\left(\sum_{i=j}^{k} \nu_i\right)^{-s_j} = D_j \exp\left(-u_j \sum_{i=j}^{k} \nu_i\right), \quad D_j := \left(-\frac{d}{du_j}\right)^{-s_j} \Bigg|_{u_j=0}.$$

Consequently,

$$\begin{aligned} \lambda\binom{s_1, \ldots, s_k}{b_1, \ldots, b_k} &= \prod_{j=1}^{k} \sum_{\nu_j=1}^{\infty} b_j^{-\nu_j} D_j \exp\left(-u_j \sum_{i=j}^{k} \nu_i\right) \\ &= \prod_{j=1}^{k} D_j \sum_{\nu_j=1}^{\infty} b_j^{-\nu_j} \exp\left(-\nu_j \sum_{i=1}^{j} u_i\right) \\ &= \prod_{j=1}^{k} D_j \left\{ \frac{1}{b_j \exp\left(\sum_{i=1}^{j} u_i\right) - 1} \right\}. \end{aligned} \tag{10}$$

In particular, (10) implies

$$\lambda\binom{0, \ldots, 0}{b_1, \ldots, b_k} = \prod_{j=1}^{k} \frac{1}{b_j - 1}. \tag{11}$$

Despite its utter simplicity, (11) points the way to deeper waters. For example, if we put $b_j = q^{-j}$ for each $j = 1, 2, \ldots, k$ and note that

$$\lambda\binom{0, 0, \ldots, 0}{q^{-1}, q^{-2}, \ldots, q^{-k}} = \sum_{n_1 > n_2 > \cdots > n_k > 0} \prod_{j=1}^{k} q^{n_j}, \quad k > 0,$$

then (11) implies the generating function equality

$$\sum_{k=0}^{\infty} z^k \lambda\binom{0, 0, \ldots, 0}{q^{-1}, q^{-2}, \ldots, q^{-k}} = \prod_{n=1}^{\infty} (1 + zq^n) = \sum_{k=0}^{\infty} z^k \prod_{j=1}^{k} \frac{q^j}{1 - q^j},$$

which experts in the field of basic hypergeometric series will recognize as a q-analogue of the exponential function and a special case of the q-binomial theorem, usually expressed in the more familiar form [25] as

$$(-zq; q)_\infty = \sum_{k=0}^{\infty} \frac{q^{k(k+1)/2}}{(q; q)_k} z^k.$$

The case $k=1$, $b_1=2$, $s_1=-n$ of (10) yields the numbers [41] (A000629)

$$\delta(-n)=\lambda_2(-n)=\sum_{k=1}^{\infty}\frac{k^n}{2^k}=\mathrm{Li}_{-n}(\tfrac{1}{2}),\quad n\ge 0, \tag{12}$$

which enumerate [33] the combinations of a simplex lock having n buttons, and which satisfy the recurrence

$$\delta(-n)=1+\sum_{j=0}^{n-1}\binom{n}{j}\delta(-j),\quad n\ge 1.$$

Also, from the exponential generating function

$$\sum_{n=0}^{\infty}\delta(-n)\frac{x^n}{n!}=\frac{e^x}{2-e^x}=\frac{2}{2-e^x}-1,$$

we infer [26, 42] that for $n\ge 1$, $\frac{1}{2}\delta(-n)$ also counts

i) the number of ways of writing a sum on n indices;

ii) the number of functions $f:\{1,2,\dots,n\}\to\{1,2,\dots,n\}$ such that if j is in the range of f, then so is each value less than or equal to j;

iii) the number of asymmetric generalized weak orders on $\{1,2,\dots,n\}$;

iv) the number of ordered partitions (preferential arrangements) of $\{1,2,\dots,n\}$.

The numbers $\frac{1}{2}\delta(-n)$ also arise [17] in connection with certain constants related to the Laurent coefficients of the Riemann zeta function. See [41] (A000670) for additional references.

3 Reductions

Given the multidimensional polylogarithm (1), we define the *depth* to be k, and the *weight* to be $s:=s_1+\cdots+s_k$. We would like to know which sums can be expressed in terms of lower depth sums. When a sum can be so expressed, we say it *reduces.* Especially interesting are the sums which completely reduce, i.e. can be expressed in terms of depth-1 sums. We say such sums *evaluate.* The concept of weight is significant, as all our reductions preserve it. More specifically, we'll see that all our reductions take the form of a polynomial expression which is homogeneous with respect to weight.

There are certain sums which cannot be expressed (polynomially) in terms of lower depth sums. Such sums are called *irreducible.* Proving irreducibility is currently beyond the reach of number theory. In particular, proving the irrationality of $\zeta(5)$ remains an open problem.

3.1 Examples of Reductions at Specific Depths

The functional equation (an example of a "stuffle" – see Sections 5.1 through 5.3)

$$\zeta(s)\zeta(t) = \zeta(s,t) + \zeta(t,s) + \zeta(s+t)$$

reduces $\zeta(s,s)$.

Broadhurst, using high-precision arithmetic and integer relations finding algorithms, has found many conjectured[2] reductions. One example is

$$\zeta(4,1,3) \stackrel{?}{=} -\zeta(5,3) + \tfrac{71}{36}\zeta(8) - \tfrac{5}{2}\zeta(5)\zeta(3) + \tfrac{1}{2}\zeta(3)^2\zeta(2), \tag{13}$$

expressing a multiple zeta value of depth three and weight eight in terms of lower depth MZVs. Observe that the combined weight of each term in the reduction is preserved. Broadhurst also noted that although $\zeta(4,2,4,2)$ is apparently irreducible in terms of lower depth MZVs, we have the conjectured weight-12 reduction

$$\begin{aligned}\zeta(4,2,4,2) \stackrel{?}{=}\ & -\tfrac{1024}{27}\lambda(9-,3) - \tfrac{267991}{5528}\zeta(12) - \tfrac{1040}{27}\zeta(9,3) - \tfrac{76}{3}\zeta(9)\zeta(3) \\ & -\tfrac{160}{9}\zeta(7)\zeta(5) + 2\zeta(6)\zeta(3)^2 + 14\zeta(5,3)\zeta(4) \\ & +70\zeta(5)\zeta(4)\zeta(3) - \tfrac{1}{6}\zeta(3)^4 \end{aligned} \tag{14}$$

in terms of lower depth MZVs *and* the alternating Euler sum $\lambda(9-,3)$. Thus, alternating Euler sums enter quite naturally into the analysis. And once the alternating sums are admitted, we shall see that more general polylogarithmic sums are required.

We remark that the depth-two sums in (14), namely $\lambda(9-,3)$, $\zeta(9,3)$, and $\zeta(5,3)$, are almost certainly irreducible. For example, if there are integers c_1, c_2, c_3, c_4 (not all equal to 0) such that $c_1\zeta(5,3) + c_2\pi^8 + c_3\zeta(3)^2\zeta(2) + c_4\zeta(5)\zeta(3) = 0$, then the Euclidean norm of the vector (c_1, c_2, c_3, c_4) is greater than 10^{50}. This result can be proved computationally in a mere 0.2 seconds on a DEC Alpha workstation using D. Bailey's fast implementation of the integer relation algorithm PSLQ [22], once we know the four input values at the precision of 200 decimal digits. Such evaluation poses no obstacle to our fast method of evaluating polylogs using the Hölder convolution (see Section 7).

3.2 An Arbitrary Depth Reduction

In contrast to the specific numerical results provided by (13) and (14), reducibility results for arbitrary sets of arguments can be obtained if one is prepared to consider certain specific combinations of MZVs. The following result is typical in this respect. It states that, depending on the parity of the depth, either the sum or the difference of

[2] Both (13) and (14) hold to at least 7900 significant figures.

an MZV with its reversed-string counterpart always reduces. Additional reductions, such as those alluded to in Sections 1 and 2, must await the development of the theory provided in Sections 4–7.

Theorem 1 *Let k be a positive integer and let $s_1, s_2, \ldots, s_k$ be positive integers with s_1 and s_k greater than 1. Then the expression*

$$\zeta(s_1, s_2, \ldots, s_k) + (-1)^k \zeta(s_k, \ldots, s_2, s_1)$$

reduces to lower depth MZVs.

Remark. The condition on s_1 and s_k is imposed only to ensure convergence of the requisite sums.

Proof. To fix ideas, suppose $k = 3$. Let $N := (\mathbf{Z}^+)^3 = \mathbf{Z}^+ \times \mathbf{Z}^+ \times \mathbf{Z}^+$ denote the Cartesian product of three copies of the positive integers. Define an additive weight-function $w : 2^N \to \mathbf{R}$ by

$$w(A) := \sum_{(n_1,n_2,n_3)\in A} n_1^{-s_1} n_2^{-s_2} n_3^{-s_3}.$$

Now if

$$\begin{aligned} P_1 &:= \{(n_1, n_2, n_3) \in N : n_1 \le n_2\}, \\ P_2 &:= \{(n_1, n_2, n_3) \in N : n_2 \le n_3\}, \end{aligned}$$

then

$$P_1 \cap P_2 = \{\vec{n} \in N : n_1 \le n_2 \le n_3\}$$

and

$$(N \setminus P_1) \cap (N \setminus P_2) = \{\vec{n} \in N : n_1 > n_2 > n_3\}.$$

By the Inclusion-Exclusion Principle,

$$w((N \setminus P_1) \cap (N \setminus P_2)) = w(N) - w(P_1) - w(P_2) + w(P_1 \cap P_2),$$

which is to say that

$$\begin{aligned} \zeta(s_1, s_2, s_3) &= \zeta(s_1)\zeta(s_2)\zeta(s_3) - \zeta(s_3)[\zeta(s_2, s_1) + \zeta(s_2 + s_1)] \\ &- \zeta(s_1)[\zeta(s_3, s_2) + \zeta(s_3 + s_2)] + \zeta(s_3 + s_2, s_1) \\ &+ \zeta(s_3, s_2 + s_1) + \zeta(s_3 + s_2 + s_1) + \zeta(s_3, s_2, s_1), \end{aligned}$$

i.e. $\zeta(s_1, s_2, s_3) - \zeta(s_3, s_2, s_1)$ reduces.

In general, let k be a positive integer and let $N := (\mathbf{Z}^+)^k$ denote the Cartesian product of k copies of the positive integers. Our additive weight-function $w : 2^N \to \mathbf{R}$ is now given by

$$w(A) := \sum_{\vec{n} \in A} \prod_{j=1}^{k} n_j^{-s_j}.$$

For each $1 \le j \le k-1$, define the subset P_j of N by

$$P_j := \{\vec{n} \in N : n_j \le n_{j+1}\}.$$

The Inclusion-Exclusion Principle states that

$$w\left(\bigcap_{j=1}^{k-1} N \setminus P_j\right) = \sum_{T \subseteq \{1,2,\ldots,k-1\}} (-1)^{|T|}\, w\left(\bigcap_{j \in T} P_j\right). \tag{15}$$

We remark that the term on the right-hand side of (15) arising from the subset $T = \{\}$ is $\zeta(s_1)\zeta(s_2)\cdots\zeta(s_k)$ by the usual convention for intersection over an empty set. Next, note that the left-hand side of (15) is simply $\zeta(s_1, s_2, \ldots, s_k)$. Finally, observe that all terms on the right-hand side of (15) have depth strictly less than k – except when $T = \{1, 2, \ldots, k-1\}$, which gives

$$(-1)^{k-1} \sum_{n_1 \le n_2 \le \cdots \le n_k} \prod_{j=1}^{k} n_j^{-s_j} = (-1)^{k-1}\zeta(s_k, \ldots, s_2, s_1) \ + \ \text{lower depth MZVs}.$$

This latter observation completes the proof of Theorem 1. $\square$

4 Integral Representations

Writing the definition of the gamma function [39] in the form

$$r^{-s}\Gamma(s) = \int_1^\infty (\log x)^{s-1} x^{-r-1}\, dx, \quad r > 0, \quad s > 0,$$

it follows that if each $s_j > 0$ and each $|b_j| \ge 1$, then

$$\begin{aligned} \lambda\binom{s_1, \ldots, s_k}{b_1, \ldots, b_k} &= \prod_{j=1}^{k} \sum_{\nu_j=1}^{\infty} b_j^{-\nu_j} \left(\sum_{i=j}^{k} \nu_i\right)^{-s_j} \\ &= \sum_{\nu_1=1}^{\infty} b_1^{-\nu_1} \frac{1}{\Gamma(s_1)} \int_1^\infty dx (\log x)^{s_1-1} x^{-\nu_1-1} \prod_{j=2}^{k} (b_j x)^{-\nu_j} \left(\sum_{i=j}^{k} \nu_i\right)^{-s_j} \\ &= \frac{1}{\Gamma(s_1)} \int_1^\infty \frac{(\log x)^{s_1-1}}{b_1 x - 1} \lambda\binom{s_2, \ldots, s_k}{b_2 x, \ldots, b_k x} \frac{dx}{x}, \end{aligned} \tag{16}$$

a representation vaguely remindful of the integral recurrence for the polylogarithm. Repeated application of (16) yields the k-dimensional integral representation

$$\lambda\binom{s_1,\ldots,s_k}{b_1,\ldots,b_k} = \prod_{j=1}^{k} \frac{1}{\Gamma(s_j)} \int_1^\infty \frac{(\log x_j)^{s_j-1} dx_j}{\left(b_j \prod_{i=1}^{j} x_i - 1\right) x_j}, \tag{17}$$

which generalizes Crandall's integral [15] for $\zeta(s_1,\ldots,s_k)$. An equivalent formulation of (17) is

$$\lambda\binom{s_1,\ldots,s_k}{b_1,\ldots,b_k} = \prod_{j=1}^{k} \frac{1}{\Gamma(s_j)} \int_0^\infty \frac{u_j^{s_j-1}\, du_j}{b_j \exp\left(\sum_{i=1}^{j} u_i\right) - 1}, \tag{18}$$

the integral transforms in (18) replacing the derivatives in (10).

Although *depth-dimensional integrals* such as (17) and (18) are attractive, they are not particularly useful. As mentioned previously, we are interested in reducing the depth whenever this is possible. However, since the weight is an invariant of all known reductions, we seek integral representations which respect weight invariance. As we next show, this can be accomplished by selectively removing logarithms from the integrand of (17), at the expense of increasing the number of integrations. At the extreme, the representation (17) is replaced by a *weight-dimensional integral* of a rational function.

4.1 The Partition Integral

We begin with the parameters in (1). Let $R_1, R_2, \ldots, R_n$ be a (disjoint) set partition of $\{1, 2, \ldots, k\}$. Put

$$r_m := \sum_{i\in R_m} s_i, \quad 1 \le m \le n.$$

If $d_1, d_2, \ldots, d_n$ are real numbers satisfying $|d_m| \ge 1$ for all m and $r_1 d_1 \ne 1$, then

$$\begin{aligned}
\lambda\binom{r_1,\ldots,r_n}{d_1,\ldots,d_n} &= \prod_{m=1}^{n} \sum_{\nu_m=1}^{\infty} d_m^{-\nu_m} \left(\sum_{j=m}^{n} \nu_j\right)^{-r_m} \\
&= \prod_{m=1}^{n} \sum_{\nu_m=1}^{\infty} d_m^{-\nu_m} \prod_{i\in R_m} \left(\sum_{j=m}^{n} \nu_j\right)^{-s_i} \\
&= \prod_{m=1}^{n} \sum_{\nu_m=1}^{\infty} d_m^{-\nu_m} \prod_{i\in R_m} \frac{1}{\Gamma(s_i)} \int_1^\infty \frac{(\log x)^{s_i-1}\, dx}{x^{1+\nu_m+\cdots+\nu_n}}.
\end{aligned}$$

Now collect bases with like exponents and note that "$\prod_{m=1}^{n} \prod_{i\in R_m} = \prod_{j=1}^{k}$." It follows that

$$\lambda\binom{r_1,\ldots,r_n}{d_1,\ldots,d_n} = \left\{\prod_{j=1}^{k} \int_1^\infty \frac{(\log x_j)^{s_j-1}\, dx_j}{\Gamma(s_j)\, x_j}\right\} \prod_{m=1}^{n} \sum_{\nu_m=1}^{\infty} d_m^{-\nu_m} \prod_{j=1}^{m} \prod_{i\in R_j} x_i^{-\nu_m}$$

$$= \left\{ \prod_{j=1}^{k} \int_1^\infty \frac{(\log x_j)^{s_j-1}\, dx_j}{\Gamma(s_j)\, x_j} \right\} \prod_{m=1}^{n} \left(d_m \prod_{j=1}^{m} \prod_{i \in R_j} x_i - 1 \right)^{-1}, \quad (19)$$

on summing the n geometric series.

EXAMPLE 4.1.1. Taking $n = k$, we have $R_m = \{m\}$, and $r_m = s_m$ for all $1 \le m \le n$. In this case, (19) reduces to the depth-dimensional integral representation (17).

EXAMPLE 4.1.2. Taking $n = 1$, we have $R_1 = \{1, 2, \ldots, k\}$ and $r_1 = s = \sum_{j=1}^k s_i$. If we also put $d := \prod_{j=1}^k d_j$, then (19) yields the seemingly wasteful k-dimensional integral

$$\lambda\binom{s}{d} = \lambda\binom{\sum_{j=1}^k s_j}{\prod_{j=1}^k d_j} = \left\{ \prod_{j=1}^{k} \int_1^\infty \frac{(\log x_j)^{s_j-1}\, dx_j}{\Gamma(s_j)\, x_j} \right\} \left(\prod_{j=1}^{k} d_j x_j - 1 \right)^{-1}$$

for a polylogarithm of depth one.

EXAMPLE 4.1.3. Let $s_1 = s_2 = \ldots = s_k = 1$, $r_0 = 0$ and for $1 \le m \le n$, put $R_m := \{(\sum_{i=1}^{m-1} r_i) + 1, (\sum_{i=1}^{m-1} r_i) + 2, \ldots, (\sum_{i=1}^{m-1} r_i) + r_m\}$, where $r_1, r_2, \ldots, r_n$ are arbitrary positive integers with $\sum_{m=1}^n r_m = k$. In this case, (19) yields a weight-dimensional integral of a rational function in k variables:

$$\lambda\binom{r_1, \ldots, r_n}{d_1, \ldots, d_n} = \left\{ \prod_{j=1}^{r_1+\cdots+r_n} \int_1^\infty \frac{dx_j}{x_j} \right\} \prod_{m=1}^{n} \left(d_m \prod_{i=1}^{r_1+\cdots+r_m} x_i - 1 \right)^{-1}. \quad (20)$$

An interesting specialization of (20) is

$$\zeta(2,1) = \int_1^\infty \int_1^\infty \int_1^\infty \frac{dx\, dy\, dz}{xyz(xy-1)(xyz-1)} = \int_1^\infty \int_1^\infty \int_1^\infty \frac{dx\, dy\, dz}{xyz(xyz-1)} = \zeta(3).$$

Although it may seem wasteful, as in Example 4.1.2 above, to use more integrations than are required, nevertheless such a technique allows an easy comparison of multi-dimensional polylogarithms having a common weight but possessing widely differing depths. For example, from the four equations

$$\begin{aligned}
\lambda\binom{s+t}{ab} &= \frac{1}{\Gamma(s)\Gamma(t)} \int_1^\infty \int_1^\infty \frac{(\log x)^{s-1} (\log y)^{t-1}\, dx\, dy}{(abxy-1)xy}, \\
\lambda\binom{s, t}{a, ab} &= \frac{1}{\Gamma(s)\Gamma(t)} \int_1^\infty \int_1^\infty \frac{(\log x)^{s-1} (\log y)^{t-1}\, dx\, dy}{(ax-1)(abxy-1)xy}, \\
\lambda\binom{t, s}{b, ab} &= \frac{1}{\Gamma(s)\Gamma(t)} \int_1^\infty \int_1^\infty \frac{(\log x)^{s-1} (\log y)^{t-1}\, dx\, dy}{(by-1)(abxy-1)xy}, \\
\lambda\binom{s}{a}\lambda\binom{t}{b} &= \frac{1}{\Gamma(s)\Gamma(t)} \int_1^\infty \int_1^\infty \frac{(\log x)^{s-1} (\log y)^{t-1}\, dx\, dy}{(ax-1)(by-1)xy}, \quad (21)
\end{aligned}$$

and the rational function identity

$$\frac{1}{(ax-1)(by-1)} = \frac{1}{abxy-1}\left(\frac{1}{ax-1}+\frac{1}{by-1}+1\right), \tag{22}$$

the "stuffle" identity (see Section 5.1)

$$\lambda\binom{s}{a}\lambda\binom{t}{b} = \lambda\binom{s,t}{a,ab}+\lambda\binom{t,s}{b,ab}+\lambda\binom{s+t}{ab} \tag{23}$$

follows immediately. The connection between "stuffle" identities and rational functions will be explained and explored more fully in Section 5.3.

4.2 The Iterated Integral

A second approach to removing the logarithms from (17) yields a weight-dimensional iterated integral. The advantage here is that the rational function comprising the integrand is particularly simple.

We use the notation of Kassel [32] for iterated integrals. For $j = 1, 2, \ldots, n$, let $f_j : [a, c] \to \mathbf{R}$ and $\Omega_j := f_j(y_j)\, dy_j$. Then

$$\begin{aligned} \int_a^c \Omega_1\Omega_2\cdots\Omega_n \quad &:= \quad \prod_{j=1}^{n}\int_a^{y_{j-1}} f_j(y_j)\, dy_j, \quad y_0 := c \\ &= \quad \begin{cases} \int_a^c f_1(y_1)\int_a^{y_1}\Omega_2\cdots\Omega_n\, dy_1 & \text{if } n>0 \\ 1 & \text{if } n=0. \end{cases} \end{aligned}$$

For each real number b, define a differential 1-form

$$\omega_b := \omega(b) := \frac{dx}{x-b}.$$

With this definition, the change of variable $y \mapsto 1-y$ generates an involution $\omega(b) \mapsto \omega(1-b)$. By repeated application of the self-evident representation

$$b^m m^{-s} = \int_0^b \omega_0^{s-1} y^{m-1}\, dy, \quad m = 1, 2, 3, \ldots$$

one derives from (1) that

$$\begin{aligned} \lambda\binom{s_1,\ldots,s_k}{b_1,\ldots,b_k} \quad &= \quad \prod_{j=1}^{k}\sum_{\nu_j=1}^{\infty} b_j^{-\nu_j}\int_0^{y_{j-1}} \omega_0^{s_j-1} y_j^{\nu_j-1}\, dy_j, \quad y_0 := 1 \\ &= \quad \prod_{j=1}^{k}\int_0^{y_{j-1}} \omega_0^{s_j-1}\frac{b_j^{-1}\, dy_j}{1-b_j^{-1}y_j} \\ &= \quad (-1)^k\int_0^1 \prod_{j=1}^{k}\omega_0^{s_j-1}\omega(b_j). \end{aligned} \tag{24}$$

Letting $s := s_1 + s_2 + \cdots + s_k$ denote the weight, one observes that the representation (24) is an s-dimensional iterated integral over the simplex $1 > y_1 > y_2 > \cdots > y_s > 0$. Scaling by q at each level yields the following version of the linear change of variable formula for iterated integrals:

$$\lambda_q\binom{s_1,\dots,s_k}{b_1,\dots,b_k} := \lambda\binom{s_1,\dots,s_k}{qb_1,\dots,qb_k} = (-1)^k \int_0^{1/q} \prod_{j=1}^k \omega_0^{s_j-1}\omega(b_j) \tag{25}$$

for any real number $q \neq 0$.

Having seen that every multidimensional polylogarithm can be represented (24) by a weight-dimensional iterated integral, it is natural to ask whether the converse holds. In fact, any convergent iterated integral of the form

$$\int_0^1 \prod_{r=1}^s \omega_{\alpha(r)} \tag{26}$$

can always (by collecting adjacent ω_0 factors – note that for convergence, $\alpha(s) \neq 0$) be written in the form

$$\int_0^1 \prod_{j=1}^k \omega_0^{s_j-1}\omega(b_j) = (-1)^k \lambda\binom{s_1,\dots,s_k}{b_1,\dots,b_k}, \tag{27}$$

where

$$0 \neq b_j = \alpha\left(\sum_{i=1}^j s_i\right). \tag{28}$$

We remark that the iterated integral representation (24) and the weight-dimensional non-iterated integral representation (20) of Example 4.1.3 are equivalent under the change of variable $x_j = y_{j-1}/y_j$, $j = 1, 2, \dots, s$, $y_0 := 1$. In fact, every integral representation of Section 4.1 has a corresponding iterated integral representation under the aforementioned transformation. For example, Crandall's integral (17) becomes

$$\lambda\binom{s_1,\dots,s_k}{b_1,\dots,b_k} = \prod_{j=1}^k \int_0^{y_{j-1}} \frac{(\log(y_{j-1}/y_j))^{s_j-1}\, dy_j}{\Gamma(s_j)(b_j - y_j)}.$$

The explicit observation that MZVs are values of iterated integrals is apparently due to Maxim Kontsevich [44]. Less formally, such representations go as far back as Euler.

5 Shuffles and Stuffles

Although it is natural to study multidimensional polylogarithmic sums as analytic objects, a good deal can be learned from the combinatorics of how they behave with respect to their argument strings.

5.1 The Stuffle Algebra

Given two argument strings $\vec{s} = (s_1, \ldots, s_k)$ and $\vec{t} = (t_1, \ldots, t_r)$, we define the set stuffle$(\vec{s}, \vec{t})$ as the smallest set of strings over the alphabet

$$\{s_1, \ldots, s_k, t_1, \ldots, t_r, \text{“+”}, \text{“,”}, \text{“(”}, \text{“)”}\}$$

satisfying

(i) $(s_1, \ldots, s_k, t_1, \ldots, t_r) \in \text{stuffle}(\vec{s}, \vec{t})$,

(ii) If a string of the form (U, s_n, t_m, V) is in stuffle$(\vec{s}, \vec{t})$, then so are the strings (U, t_m, s_n, V) and $(U, s_n + t_m, V)$.

Let $\vec{a} = (a_1, \ldots, a_k)$ and $\vec{b} = (b_1, \ldots, b_r)$ be two strings of the same length as $\vec{s}$ and $\vec{t}$, respectively. We now define

$$ST := ST\binom{\vec{s}, \vec{t}}{\vec{a}, \vec{b}} \tag{29}$$

to be the set of all pairs $\binom{\vec{u}}{\vec{c}}$ with $\vec{u} \in \text{stuffle}(\vec{s}, \vec{t})$ and $\vec{c} = (c_1, c_2, \ldots, c_h)$ defined as follows:

i) h is the number of components of $\vec{u}$,

ii) $c_0 := a_0 := b_0 := 1$,

iii) for $1 \le j \le h$, if $c_{j-1} = a_{n-1}b_{m-1}$, then

$$c_j := \begin{cases} a_n b_m, & \text{if } u_j = s_n + t_m, \\ a_n b_{m-1}, & \text{if } u_j = s_n, \\ a_{n-1} b_m, & \text{if } u_j = t_m. \end{cases}$$

5.2 Stuffle Identities

A class of identities which we call *“depth-length shuffles”* or *“stuffle identities”* is generated by a formula for the product of two λ-functions. Consider

$$\lambda\binom{\vec{s}}{\vec{a}}\lambda\binom{\vec{t}}{\vec{b}} = \left\{\prod_{j=1}^{k}\sum_{\nu_j=1}^{\infty} a_j^{-\nu_j}\left(\sum_{i=j}^{k}\nu_i\right)^{-s_j}\right\}\left\{\prod_{j=1}^{r}\sum_{\xi_j=1}^{\infty} b_j^{-\xi_j}\left(\sum_{i=j}^{r}\xi_i\right)^{-t_j}\right\}.$$

If we put

$$n_j := \textstyle\sum_{i=j}^{k}\nu_i, \quad m_j := \sum_{i=j}^{r}\xi_i,$$
$$a_j := \textstyle\prod_{i=1}^{j} x_i, \quad b_j := \prod_{i=1}^{j} y_i,$$

then it follows that

$$\lambda\binom{\vec{s}}{\vec{a}}\lambda\binom{\vec{t}}{\vec{b}} = \sum_{\substack{n_1 > \cdots > n_k > 0 \\ m_1 > \cdots > m_r > 0}} \left(\prod_{j=1}^{k} x_j^{-n_j} n_j^{-s_j}\right)\left(\prod_{j=1}^{r} y_j^{-m_j} m_j^{-t_j}\right).$$

Rewriting the previous expression in terms of λ-functions yields the stuffle formula

$$\lambda\binom{\vec{s}}{\vec{a}}\lambda\binom{\vec{t}}{\vec{b}} = \sum \lambda\binom{\vec{u}}{\vec{c}}, \tag{30}$$

where the sum is over all pairs of strings $\binom{\vec{u}}{\vec{c}} \in ST\binom{\vec{s},\vec{t}}{\vec{a},\vec{b}}$.

EXAMPLE 5.2.1.

$$\lambda\binom{r,s}{a,b}\lambda\binom{t}{c} = \lambda\binom{r,s,t}{a,b,bc} + \lambda\binom{r,s+t}{a,bc} + \lambda\binom{r,t,s}{a,ac,bc} + \lambda\binom{r+t,s}{ac,bc} + \lambda\binom{t,r,s}{c,ac,bc}.$$

When specialized to MZVs, this example produces the identity

$$\zeta(r,s)\zeta(t) = \zeta(r,s,t) + \zeta(r,s+t) + \zeta(r,t,s) + \zeta(r+t,s) + \zeta(t,r,s).$$

The term "stuffle" derives from the manner in which the two (upper) strings are combined. The relative order of the two strings is preserved (shuffles), but elements of the two strings may also be shoved together into a common slot (stuffing), thereby reducing the depth.

5.3 Stuffles and Partition Integrals

In Section 4.1, an example was given in which a stuffle identity (23) was seen to arise from a corresponding rational function identity (22) and certain partition integral representations (21). This is by no means an isolated phenomenon. In fact, we shall show that *every* stuffle identity is a consequence of the partition integral (19) applied to a corresponding rational function identity.

Theorem 2 *Every stuffle identity is equivalent to a rational function identity, via the partition integral.*

Before proving Theorem 2, we define a class of rational functions, and prove they satisfy a certain rational function identity. Let $\vec{s} = (s_1, \ldots, s_k)$, $\vec{\alpha} = (\alpha_1, \ldots, \alpha_k)$, $\vec{t} = (t_1, \ldots, t_r)$, and $\vec{\beta} = (\beta_1, \ldots, \beta_r)$ be vectors of indeterminates. As in (29), put

$$ST = ST\binom{\vec{s},\vec{t}}{\vec{\alpha},\vec{\beta}},$$

and define

$$T = T(\vec{\alpha}, \vec{\beta}) := \{\vec{\gamma} : \binom{\vec{u}}{\vec{\gamma}} \in ST\}.$$

Let $f : T \to \mathbf{Q}[\gamma_1, \gamma_2, \ldots]$ be defined by

$$f(\gamma_1, \ldots, \gamma_h) := \prod_{j=1}^{h} (\gamma_j - 1)^{-1}. \tag{31}$$

Then we have the following lemma.

Lemma 1 *Let f be defined as in (31). Then*

$$f(\vec{\alpha})f(\vec{\beta}) = \sum_{\vec{\gamma} \in T(\vec{\alpha}, \vec{\beta})} f(\vec{\gamma}).$$

Proof of Lemma 1. Apply (30) with $\vec{a} = \vec{\alpha}$ and $\vec{b} = \vec{\beta}$. In view of (11), the lemma follows on taking $\vec{s}$ and $\vec{t}$ to be zero vectors of the appropriate lengths. □

Proof of Theorem 2. Let $\vec{s}$, $\vec{t}$, $\vec{a}$, and $\vec{b}$ be as in (30). Let $\vec{\alpha}$ and $\vec{\beta}$ be given by

$$\alpha_j := a_j \prod_{i=1}^{j} x_i, \quad \beta_j := b_j \prod_{i=1}^{j} y_i.$$

Applying Lemma 1 and the partition integral representation (19) to Crandall's integral (17) yields

$$\begin{aligned}
\lambda\binom{\vec{s}}{\vec{a}}\lambda\binom{\vec{t}}{\vec{b}} &= \left\{\prod_{j=1}^{k}\int_1^\infty \frac{(\log x_j)^{s_j-1}dx_j}{\Gamma(s_j)\,x_j}\right\} f(\vec{\alpha}) \left\{\prod_{j=1}^{r}\int_1^\infty \frac{(\log y_j)^{t_j-1}dy_j}{\Gamma(s_j)\,y_j}\right\} f(\vec{\beta}) \\
&= \left\{\prod_{j=1}^{k}\int_1^\infty \frac{(\log x_j)^{s_j-1}dx_j}{\Gamma(s_j)\,x_j}\right\} \left\{\prod_{j=1}^{r}\int_1^\infty \frac{(\log y_j)^{t_j-1}dy_j}{\Gamma(s_j)\,y_j}\right\} \sum_{\vec{\gamma} \in T(\vec{\alpha},\vec{\beta})} f(\vec{\gamma}) \\
&= \sum_{\vec{\gamma} \in T(\vec{\alpha},\vec{\beta})} \left\{\prod_{j=1}^{k}\int_1^\infty \frac{(\log x_j)^{s_j-1}dx_j}{\Gamma(s_j)\,x_j}\right\} \left\{\prod_{j=1}^{r}\int_1^\infty \frac{(\log y_j)^{t_j-1}dy_j}{\Gamma(s_j)\,y_j}\right\} f(\vec{\gamma}) \\
&= \sum_{\binom{\vec{u}}{\vec{c}} \in ST\binom{\vec{s},\vec{t}}{\vec{a},\vec{b}}} \lambda\binom{\vec{u}}{\vec{c}},
\end{aligned}$$

as required. □

5.4 The Shuffle Algebra

As opposed to depth-length shuffles, or stuffles, which arise from the definition (1) in terms of sums, the iterated integral representation (24) gives rise to what are called em "weight-length shuffles", or simply "shuffles". Weight-length shuffles take the form

$$\int_0^1 \Omega_1\Omega_2\cdots\Omega_n \int_0^1 \Omega_{n+1}\Omega_{n+2}\cdots\Omega_{n+m} = \sum \int_0^1 \Omega_{\sigma(1)}\Omega_{\sigma(2)}\cdots\Omega_{\sigma(n+m)}, \tag{32}$$

where the sum is over all $\binom{n+m}{n}$ permutations σ of the set $\{1, 2, \ldots, n+m\}$ which satisfy $\sigma^{-1}(i) < \sigma^{-1}(j)$ for all $1 \le i < j \le n$ and $n+1 \le i < j \le n+m$. In other words, the sum is over all $(n+m)$-dimensional iterated integrals in which the relative orders of the two strings of 1-forms $\Omega_1, \ldots, \Omega_n$ and $\Omega_{n+1}, \ldots, \Omega_{n+m}$ are preserved.

EXAMPLE 5.4.1.

$$\begin{aligned}
\zeta(2,1)\zeta(2) &= -\int_0^1 \omega_0\omega_1^2 \int_0^1 \omega_0\omega_1 \\
&= -6\int_0^1 \omega_0^2\omega_1^3 - 3\int_0^1 \omega_0\omega_1\omega_0\omega_1^2 - \int_0^1 \omega_0\omega_1^2\omega_0\omega_1 \\
&= 6\zeta(3,1,1) + 3\zeta(2,2,1) + \zeta(2,1,2).
\end{aligned}$$

In contrast, the stuffle formula gives

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

Note that weight-length shuffles preserve both depth and weight. In other words, the depth (weight) of each term which occurs in the sum over shuffles is equal to the combined depth (weight) of the two multidimensional polylogarithms comprising the product.

6 Duality

In [28], Hoffman defines an involution on strings $s_1, \ldots, s_k$. The involution coincides with a notion we refer to as duality. The duality principle states that two MZVs coincide whenever their argument strings are dual to each other, and (as noted by Zagier [44]) follows readily from the iterated integral representation. In [10], Broadhurst generalized the notion of duality to include relations between iterated integrals involving the sixth root of unity; here we allow arbitrary complex values of b_j. Thus, we find that the duality principle easily extends to multidimensional polylogarithms, and in this more general setting, has far-reaching implications.

6.1 Duality for Multidimensional Polylogarithms

We begin with the iterated integral representation (24) of Section 4.2. Reversing the order of the omegas and replacing each integration variable y by its complement $1-y$ yields the dual iterated integral representation

$$\lambda\begin{pmatrix} s_1,\ldots,s_k \\ b_1,\ldots,b_k \end{pmatrix} = (-1)^{s+k}\int_0^1 \prod_{j=k}^{1} \omega(1-b_j)\omega_1^{s_j-1}, \tag{33}$$

where again $s = s_1 + \cdots + s_k$ is the weight.

Example 6.1.1. Using (1), (24), and (33), we have

$$\lambda\begin{pmatrix} 2,1 \\ 1,-1 \end{pmatrix} = \int_0^1 \omega(0)\,\omega(1)\,\omega(-1) = -\int_0^1 \omega(2)\,\omega(0)\,\omega(1) = -\lambda\begin{pmatrix} 1,2 \\ 2,1 \end{pmatrix},$$

which is to say that

$$\sum_{n=1}^{\infty}\frac{1}{n^2}\sum_{k=1}^{n-1}\frac{(-1)^k}{k} = -\sum_{n=1}^{\infty}\frac{1}{n2^n}\sum_{k=1}^{n-1}\frac{2^k}{k^2},$$

a result that would doubtless be difficult to prove by naïve series manipulations alone.

When $b_1 = b_2 = \ldots = b_k = b$, the two dual iterated integral representations (24) and (33) simplify as follows:

$$\lambda_b(s_1,\ldots,s_k) = (-1)^k\int_0^1 \prod_{j=1}^{k}\omega_0^{s_j-1}\omega(b) = (-1)^{s+k}\int_0^1 \prod_{j=k}^{1}\omega(1-b)\omega_1^{s_j-1}. \tag{34}$$

A somewhat more symmetric version of (34) is

$$\begin{aligned}(-1)^m\lambda_b(s_1+2,\{1\}^{r_1},\ldots,s_m+2,\{1\}^{r_m}) &= (-1)^r\int_0^1 \prod_{j=1}^{m}\omega_0^{s_j+1}\omega_b^{r_j+1} \\ &= (-1)^s\int_0^1 \prod_{j=m}^{1}\omega_{1-b}^{r_j+1}\omega_1^{s_j+1},\end{aligned} \tag{35}$$

where $r := \sum_j r_j$ and, as usual, $s := \sum_j s_j$.

6.2 Duality for Unsigned Euler Sums

Taking $b=1$ in (35), we deduce the *MZV duality formula* (cf. [32] p. 483)

$$\zeta(s_1+2,\{1\}^{r_1},\ldots,s_m+2,\{1\}^{r_m}) = \zeta(r_m+2,\{1\}^{s_m},\ldots,r_1+2,\{1\}^{s_1}) \tag{36}$$

for multidimensional unsigned Euler sums.

EXAMPLE 6.2.1. MZV duality (36) gives Euler's evaluation $\zeta(2,1) = \zeta(3)$, as well as the generalizations $\zeta(\{2,1\}^n) = \zeta(\{3\}^n)$, and $\zeta(2,\{1\}^n) = \zeta(n+2)$, valid for all nonnegative integers n.

In [40] a beautiful extension of MZV duality (36) is given, which also subsumes the so-called sum formula

$$\sum_{\substack{n_j > \delta_{j,1} \\ N=\Sigma_j n_j}} \zeta(n_1, n_2, \ldots, n_k) = \zeta(N),$$

conjectured independently by C. Moen [28] and M. Schmidt [38], and subsequently proved by A. Granville [27]. We refer the reader to Dr. Ohno's preprint for details.

The duality principle has an enticing converse, namely that *two MZVs with distinct argument strings are equal only if the argument strings are dual to each other.* Unfortunately, although the numerical (and symbolic) evidence in support of this converse statement is overwhelming, it still remains to be proved. In the case of self-dual strings, the conjectured converse of the duality principle implies that such a MZV can equal no other MZV; moreover we find that certain of these completely reduce, i.e. evaluate entirely in terms of (depth-one) Riemann zeta functions.

EXAMPLE 6.2.2. The following self-dual evaluation, previously conjectured by Don Zagier [44]

$$\zeta(\{3,1\}^n) = 4^{-n}\zeta(\{4\}^n) = \frac{2\pi^{4n}}{(4n+2)!}, \quad n \geq 0,$$

is proved herein (see Section 12).

CONJECTURE: The self-dual two-parameter generalization of the previous example

$$\zeta(\{2\}^m, \{3, \{2\}^m, 1, \{2\}^m\}^n) \stackrel{?}{=} \frac{2(m+1)\pi^{4(m+1)n+2m}}{(2(m+1)(2n+1))!}, \quad n \geq 0, \quad m \geq 0,$$

remains to be proved. Example 2.3 of Section 2 is also a conjectured self-dual evaluation.

We conclude this section with the following result, since the special case $p = 1$ has some bearing on the MZV duality formula (36).

Theorem 3 *Let $|p| \geq 1$. The double generating function equality*

$$1 - \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} x^{m+1}y^{n+1}\lambda_p(m+2,\{1\}^n) = {}_2F_1\left(\begin{matrix} y, -x \\ 1-x \end{matrix} \,\middle|\, \frac{1}{p} \right)$$

holds.

Proof. By definition (6) of λ_p,

$$\begin{aligned}
\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} x^{m+1}y^{n+1}\lambda_p(m+2,\{1\}^n) &= y\sum_{m=0}^{\infty} x^{m+1}\sum_{k=1}^{\infty}\frac{1}{k^{m+2}p^k}\prod_{j=1}^{k-1}\left(1+\frac{y}{j}\right) \\
&= \sum_{m=0}^{\infty} x^{m+1}\sum_{k=1}^{\infty}\frac{(y)_k}{k^{m+1}k!p^k} \\
&= \sum_{k=1}^{\infty}\frac{(y)_k}{k!p^k}\left(\frac{x}{k-x}\right) \\
&= -\sum_{k=1}^{\infty}\frac{(y)_k(-x)_k}{k!p^k(1-x)_k} \\
&= 1-{}_2F_1\left(\begin{array}{c} y,-x \\ 1-x \end{array}\,\middle|\,\frac{1}{p}\right)
\end{aligned}$$

as claimed. □

Remarks. In [5] it was noted that the $p=1$ case of Theorem 4 is equivalent to the $m=1$ case of MZV duality (36) via the invariance of

$$ {}_2F_1\left(\begin{array}{c} y,-x \\ 1-x \end{array}\,\middle|\,1\right) = \frac{\Gamma(1-x)\Gamma(1-y)}{\Gamma(1-x-y)} = \exp\left\{\sum_{k=2}^{\infty}\left(x^k+y^k-(x+y)^k\right)\frac{\zeta(k)}{k}\right\} \quad (37)$$

with respect to the interchange of x and y. However, it appears that this observation can be traced back to Drinfeld [18]. In connection with his work on series of Lie brackets, Drinfeld encountered a scaled version of the exponential series above, and showed that the coefficients of the double generating function satisfy $c_{mn}=c_{nm}$ and $c_{m0}=c_{0m}$ evaluates to $\zeta(m+2)$, up to a so-called Oppenheimer factor which we omit ([32], p. 468). In our notation, this is essentially the statement that $\zeta(m+2,\{1\}^n)=\zeta(n+2,\{1\}^m)$.

Note that Theorem 4 in conjunction with (37) shows that $\zeta(m+2,\{1\}^n)$ completely reduces (i.e. is expressible solely in terms of depth-1 Riemann zeta values) for all nonnegative integers m and n. In particular, the coefficient of $x^{m-1}y^2$ gives Euler's formula (Example 2.1), while the coefficient of $x^{m-1}y^3$ gives Markett's formula [38] for $\zeta(m,1,1)$, $m\geq 2$. Thus, the complete reducibility of $\zeta(m+2,\{1\}^n)$ is a simple consequence of Gauss's ${}_2F_1$ hypergeometric summation theorem (37).

It would be interesting to know if there's a generating function formulation of MZV duality at full strength (36). Presumably, it would involve an analogue of Drinfeld's associator in $2m$ non-commuting variables.

6.3 Duality for Unit Euler Sums

Recall the δ-function was defined (7) as the nested sum extension of the polylogarithm at one-half:

$$\delta(s_1,\ldots,s_k) := \lambda\begin{pmatrix} s_1,\ldots,s_k \\ 2,\ldots,2 \end{pmatrix} = \prod_{j=1}^{k}\sum_{\nu_j=1}^{\infty} 2^{-\nu_j}\left(\sum_{i=j}^{k}\nu_i\right)^{-s_j}. \tag{38}$$

Due to its geometric rate of convergence, δ-values can be computed to high precision relatively quickly. On the other hand, the unit Euler μ-sums (8) converge extremely slowly when the b_j all lie on the unit circle. In particular, the slow convergence of the unit (± 1) argument μ-sums initially confounded our efforts to create a data-base of numerical evaluations from which to form viable conjectures. Nevertheless, there is a close relationship between the δ-sums and the μ-sums, as we shall presently see.

Taking $b = 2$ in (35), we deduce the "delta-to-unit-mu" duality formula

$$\begin{aligned} &\delta(s_1+2,\{1\}^{r_1},\ldots,s_m+2,\{1\}^{r_m}) \\ &\quad = (-1)^{r+m}\mu(\{-1\}^{r_m+1},\{1\}^{s_m+1},\ldots,\{-1\}^{r_1+1},\{1\}^{s_1+1}). \end{aligned} \tag{39}$$

Thus, every convergent unit (± 1) argument μ-sum can be expressed as a (rapidly convergent) δ-sum. The converse follows from the more general, but less symmetric formula, arising from (34):

$$\delta(s_1,\ldots,s_k) = (-1)^k\mu(-1,\{1\}^{s_k-1},\ldots,-1,\{1\}^{s_1-1}). \tag{40}$$

Example 6.3.1.

$$\delta(1) = \sum_{\nu=1}^{\infty}\frac{1}{\nu 2^\nu} = -\log(\tfrac{1}{2}) = \sum_{\nu=1}^{\infty}\frac{(-1)^{\nu+1}}{\nu} = -\mu(-1),$$

and more generally, for all nonnegative integers n, we have

$$\delta(n+1) = \sum_{\nu=1}^{\infty}\frac{1}{\nu^{n+1}2^\nu} = \mathrm{Li}_{n+1}(\tfrac{1}{2}) = -\mu(-1,\{1\}^n).$$

Example 6.3.2.

$$\delta(\{1\}^n) = (-1)^n\mu(\{-1\}^n) = (\log 2)^n/n!, \quad n \ge 0, \tag{41}$$

$$\delta(2,\{1\}^n) = (-1)^{n+1}\mu(\{-1\}^{n+1},1), \quad n \ge 0, \tag{42}$$

and more generally,

$$\delta(\{1\}^m,2,\{1\}^n) = (-1)^{m+n+1}\mu(\{-1\}^{n+1},1,\{-1\}^m), \quad m \ge 0, \quad n \ge 0.$$

EXAMPLE 6.3.3.

$$\delta(1,n+1)=\mu(-1,\{1\}^n,-1),\quad n\ge 0,$$

and in particular,

$$\begin{aligned}
\delta(1,0) &= 1-\log 2,\\
\delta(1,1) &= \tfrac{1}{2}(\log 2)^2,\\
\delta(1,2) &= \tfrac{5}{7}\mathrm{Li}_2(\tfrac12)\mathrm{Li}_1(\tfrac12)-\tfrac{2}{7}\mathrm{Li}_3(\tfrac12)+\tfrac{5}{21}\left[\mathrm{Li}_1(\tfrac12)\right]^3,\\
\delta(1,3) &= \mathrm{Li}_3(\tfrac12)\mathrm{Li}_1(\tfrac12)-\tfrac12\left[\mathrm{Li}_2(\tfrac12)\right]^2.
\end{aligned}$$

Integer relation searches (see [8] or [5] for details) have failed to find a similar formula for $\delta(1,4)$. However,

$$\delta(1,-n)=\sum_{\nu=0}^{n}\binom{n}{\nu}\frac{B_{n-\nu}\delta(-\nu)}{\nu+1},\quad n\ge 1,$$

where the $\delta(-\nu)$ are the simplex lock numbers (12) and the B_ν are the Bernoulli numbers [1]. More generally, if n_1 is a positive integer and $n_2,n_3,\ldots,n_r$ are all nonnegative integers, then

$$\delta(s,-n_r,\ldots,-n_2,-n_1)=\left\{\prod_{j=1}^{r}\sum_{\nu_j=0}^{\tau_j}A(\nu_j)\right\}\delta(s-\nu_r-1),\quad s\in\mathbf{C},$$

where

$$\tau_j:=n_j+\nu_{j-1}+1,\quad A(\nu_j):=\frac{1}{\nu_j+1}\binom{\tau_j}{\nu_j}B_{\tau_j-\nu_j},\quad \nu_0:=-1.$$

7 The Hölder Convolution

We have seen how multidimensional polylogarithms with unit arguments can be expressed in terms of rapidly convergent δ-sums. What if the arguments are not necessarily units? In the iterated integral representation (24) the domain $1>y_j>y_{j+1}>0$ in $s=\sum_j s_j$ variables splits into $s+1$ parts. Each part is a product of regions $1>y_j>y_{j+1}>1/p$ for the first r variables, and $1/p>y_j>y_{j+1}>0$ for the remaining $s-r$ variables. Next, $y_j\mapsto 1-y_j$ replaces an integral of the former type by one of the latter type, with $1/p$ replaced by $1/q:=1-1/p$.

Motivated by these observations, we consider the string of differential 1-forms which occurs in the integrand of the iterated integral representation (24) and define

$$\alpha_r:=\begin{cases} b_j, & \text{if } r=\sum_{i=1}^{j}s_i\\ 0, & \text{otherwise.}\end{cases}$$

Then

$$\lambda\binom{s_1,\ldots,s_k}{b_1,\ldots,b_k} = (-1)^k \int_0^1 \prod_{r=1}^{s} \omega(\alpha_r)$$
$$= \sum_{r=0}^{s} (-1)^{r+k} \left\{ \int_0^{1/q} \prod_{j=r}^{1} \omega(1-\alpha_j) \right\} \left\{ \int_0^{1/p} \prod_{j=r+1}^{s} \omega(\alpha_j) \right\}. \quad (43)$$

Thus, by means of (26), (27), and (28), we have expressed the general multidimensional polylogarithm as a convolution of λ_p with λ_q for any p, q such that the Hölder condition $1/p + 1/q = 1$ is satisfied. For this reason, we refer to (43) as the *Hölder convolution.* Note that the Hölder convolution generalizes duality (33) for multidimensional polylogarithms, as can be seen by letting p tend to infinity so that (25) $\lambda_p \to 0$, and $q \to 1$.

MZV Example. For any $p > 0$, $q > 0$ with $1/p + 1/q = 1$,

$$\begin{aligned}\zeta(2,1,2,1,1,1) &= \lambda_p(2,1,2,1,1,1) + \lambda_p(1,1,2,1,1,1)\lambda_q(1) + \lambda_p(1,2,1,1,1)\lambda_q(2) \\ &\quad +\lambda_p(2,1,1,1)\lambda_q(3) + \lambda_p(1,1,1,1)\lambda_q(1,3) + \lambda_p(1,1,1)\lambda_q(2,3) \\ &\quad +\lambda_p(1,1)\lambda_q(3,3) + \lambda_p(1)\lambda_q(4,3) + \lambda_q(5,3) \\ &= \zeta(5,3).\end{aligned}$$

The pattern should be clear. For $1 \le j \le m$, define the concatenation products

$$\vec{a}_j := \prod_{i=j}^{m} \{s_i+2, \{1\}^{r_i}\} = \{s_j+2, \{1\}^{r_j}, \ldots, s_m+2, \{1\}^{r_m}\},$$
$$\vec{b}_j := \prod_{i=j}^{1} \{r_i+2, \{1\}^{s_i}\} = \{r_j+2, \{1\}^{s_j}, \ldots, r_1+2, \{1\}^{s_1}\},$$

and $\vec{a}_{m+1} := \vec{b}_0 := \{\}$. Then the Hölder convolution for the general MZV case is given by

$$\begin{aligned}\zeta(\vec{a}_m) &= \sum_{j=1}^{m} \left\{ \sum_{t=0}^{s_j+1} \lambda_p(s_j+2-t, \{1\}^{r_j}, \vec{a}_{j+1}) \lambda_q(\{1\}^t, \vec{b}_{j-1}) \right. \\ &\quad \left. + \sum_{\nu=1}^{r_j} \lambda_p(\{1\}^\nu, \vec{a}_{j+1}) \lambda_q(r_j+2-\nu, \{1\}^{s_j}, \vec{b}_{j-1}) \right\} + \lambda_q(\vec{b}_m) \quad (44) \\ &= \zeta(\vec{b}_m).\end{aligned}$$

Of course, $\vec{a}_m$ and $\vec{b}_m$ are the dual strings in the MZV duality formula (36). Since the sums λ_p converge geometrically, whereas MZV sums converge only polynomially, (44) provides an excellent method of computing general MZVs to high precision with the optimal parameter choice $p = q = 2$. For rapid computation of general multidimensional polylogarithms, it is simplest to use the Hölder convolution (43) directly, translating the iterated integrals into geometrically convergent sums on a case by case basis, using (24).

Alternating Example.

$$
\begin{aligned}
\lambda(2,1-) &= \int_0^1 \omega(0)\omega(1)\omega(-1)\\
&= \int_0^{1/p} \omega(0)\omega(1)\omega(-1) - \int_0^{1/q} \omega(1)\int_0^{1/p} \omega(1)\omega(-1)\\
&\quad + \int_0^{1/q} \omega(0)\omega(1)\int_0^{1/p} \omega(-1) - \int_0^{1/q} \omega(2)\omega(0)\omega(1)\\
&= \lambda_p(2,1-) + \lambda_p(1,1-)\lambda_q(1) + \lambda_p(1-)\lambda_q(2) - \lambda_q\begin{pmatrix}1,2\\2,1\end{pmatrix}\\
&= -\lambda\begin{pmatrix}1,2\\2,1\end{pmatrix}.
\end{aligned}
$$

Although we could now work out the explicit form of the analogue to (44) in the alternating case, the resulting formula is too complicated in relation to its importance to justify including here.

In addition to the impressive computational implications already outlined, the Hölder convolution (43) gives new relationships between multidimensional polylogarithms, providing a path to understanding certain previously mysterious evaluations. For example, taking $p = q = 2$ shows that every MZV of weight s can be written as a weight-homogeneous convolution sum involving $2s$ δ-functions. Furthermore, employing the weight-length shuffle formula (32) to each product shows that every MZV of weight s is a sum of 2^s (not necessarily distinct) δ-values, each of weight s, and each appearing with unit $(+1)$ coefficient. In particular, this shows that the vector space of rational linear combinations of MZVs is spanned by the set of all δ-values. Thus,

$$
\begin{aligned}
\zeta(3) &= -\int_0^{1/2} \omega_0\omega_0\omega_1 + \int_0^{1/2} \omega_1 \int_0^{1/2} \omega_0\omega_1 - \int_0^{1/2} \omega_1\omega_1 \int_0^{1/2} \omega_1 + \int_0^{1/2} \omega_0\omega_1\omega_1\\
&= \delta(3) + \int_0^{1/2} (\omega_1 \cdot \omega_0\omega_1 + \omega_0 \cdot \omega_1 \cdot \omega_1 + \omega_0\omega_1 \cdot \omega_1)\\
&\quad - \int_0^{1/2} (\omega_1\omega_1 \cdot \omega_1 + \omega_1 \cdot \omega_1 \cdot \omega_1 + \omega_1 \cdot \omega_1\omega_1) + \delta(2,1)\\
&= \delta(3) + \delta(1,2) + \delta(2,1) + \delta(2,1) + \delta(1,1,1) + \delta(1,1,1) + \delta(1,1,1) + \delta(2,1).
\end{aligned}
$$

Polylog Example. Applying (43) to $\zeta(n+2)$, with $p = q = 2$ provides a lovely closed form for $\delta(2,\{1\}^n)$. Indeed,

$$\zeta(n+2) = \delta(2,\{1\}^n) + \sum_{r=1}^{n+2} \delta(r)\delta(\{1\}^{n+2-r}). \tag{45}$$

The desired closed form follows after rearranging the previous equation (45) and applying the definition (38) and the result (41) in the form $\delta(r) = \mathrm{Li}_r(\frac{1}{2})$ and $\delta(\{1\}^r) = (\log 2)^r/r!$, respectively.

Example. Putting $n = 1$ in (45) gives [3]

$$\zeta(3) = \sum_{n=1}^{\infty} \frac{1}{n^3} = \frac{1}{12}\pi^2 \log(2) + \sum_{n=1}^{\infty} \frac{1}{2^n n^2} \sum_{j=1}^{n} \frac{1}{j}. \tag{46}$$

In fact, formula (45) is non-trivial even when $n = 0$. Putting $n = 0$ in (45) gives the classical evaluation of the dilogarithm at one-half:

$$2\mathrm{Li}_2(\tfrac{1}{2}) = \zeta(2) - (\log 2)^2 \quad \text{i.e.} \quad \sum_{n=1}^{\infty} \frac{1}{2^n n^2} = \tfrac{1}{12}\pi^2 - \tfrac{1}{2}(\log 2)^2.$$

Differentiation of (43) with respect to the parameter p provides another avenue of pursuit which has not yet been fully explored. We have used this approach to derive $\delta(0,\{1\}^n) = \delta(\{1\}^n)$, but in fact, removing the initial zero is trivial from first principles.

7.1 EZ Face

A fast program for evaluating MZVs (as well as arithmetic expressions containing them) based on the formula (44) has been developed at the CECM[3], and is available for public use via the World Wide Web interface called "EZ Face" (an abbreviation for Euler Zetas interFace) at the URL

`http://www.cecm.sfu.ca/cgi-bin/EZFace/zetaform.cgi`

This publicly accessible interface currently allows one to evaluate the sums

$$\mathtt{z}(s_1,\ldots,s_k) := \sum_{n_1>n_2>\ldots>n_k} \prod_{j=1}^{k} n_j^{-|s_j|}\sigma_j^{-n_j}$$

for non-zero integers $s_1,\ldots,s_k$ and $\sigma_j := \mathrm{signum}(s_j)$, and

$$\mathtt{zp}(p,s_1,\ldots,s_k) := \sum_{n_1>n_2>\ldots>n_k} p^{-n_1} \prod_{j=1}^{k} n_j^{-s_j}$$

[3]Centre for Experimental and Constructive Mathematics, Simon Fraser University.

for real $p \geq 1$ and positive integers $s_1, \ldots, s_k$.

The precision of the evaluation can be set anywhere between 10 and 100 digits.

Progress is currently underway to improve the implementation of alternating sums, (which are currently much less efficiently and accurately evaluated), and to extend the scope of sums that can be evaluated. The exact status of the EZ Face is at any moment documented at its “Definitions” and “Implementation Details” pages.

Additionally to the functions `z` and `zp`, the `lindep` function can be called to discover integer relations [8] between different polylog values (under the assumption that these values are known to sufficient precision). An integer relation for a vector of real numbers $(x_1, \ldots, x_n)$ is a non-zero integer vector $(c_1, \ldots, c_n)$ such that $\sum_{i=1}^{n} c_i x_i = 0$. The required syntax is `lindep`$([x_1, \ldots, x_n])$, where $x_1, \ldots, x_n$ is the vector of values for which the relation is sought.

EZ FACE EXAMPLES.

The left-aligned lines represent the input to EZ Face, while the centered lines represent the output of EZ Face. All computations are done with the precision of 50 digits.

```
Pi^6/z(6)

          945.00000000000000000000000000000000000000000000000


lindep([z(4,1,3), z(5,3), z(8), z(5)*z(3), z(3)^2*z(2)])

                        36., 36., -71., 90., -18.


lindep([ z(3), Pi^2*log(2), zp(2,2,1), zp(2,3) ])

                          12., -1., -12., -12.
```

The first example is a simple instance of Euler’s formula for $\zeta(2n)$. The second example is the discovery of equation (13). The third example confirms formula (46).

8 Evaluations for Unit Euler Sums

As usual, the Hölder conjugates p and q denote real numbers satisfying $1/p + 1/q = 1$, and $p > 1$ or $p \leq -1$ for convergence. Our first result is an easy consequence of the binomial theorem.

Theorem 4 *The generating function equality*

$$1 + \sum_{n=1}^{\infty} x^n \mu(\{p\}^n) = q^x.$$

holds.

Proof. By definition (8) of μ,

$$\begin{aligned} 1 + \sum_{n=1}^{\infty} x^n \mu(\{p\}^n) &= 1 + x \sum_{m=1}^{\infty} \frac{1}{mp^m} \prod_{j=1}^{m-1} \left(1 + \frac{x}{j}\right) \\ &= 1 + \sum_{m=1}^{\infty} \left(\frac{-1}{p}\right)^m \binom{-x}{m} \\ &= (1 - 1/p)^{-x} \\ &= q^x. \end{aligned}$$

□

Corollary 1

$$\mu(\{p\}^n) = (\log q)^n/n!, \quad n \geq 0.$$

Remarks. Of course, when $n = 0$, we need to invoke the usual empty product convention to properly interpret $\mu(\{\}) = 1$. Since the mapping $p \mapsto 1 - p$ induces the mapping $q \mapsto 1/q$ under the Hölder correspondence, duality (34) takes the particularly appealing form $\mu(\{p\}^n) = (-1)^n \mu(\{1 - p\}^n)$ in this context. In particular, $p = -1$ and δ-duality (40), (41) gives

$$\delta(\{1\}^n) = (-1)^n \mu(\{-1\}^n) = (\log 2)^n/n!, \quad n \geq 0,$$

i.e.

$$\prod_{j=1}^{n} \sum_{\nu_j=1}^{\infty} \frac{1}{2^{\nu_j}(\nu_j + \cdots + \nu_n)} = \prod_{j=1}^{n} \sum_{\nu_j=1}^{\infty} \frac{(-1)^{\nu_j+1}}{\nu_j + \cdots + \nu_n} = \frac{(\log 2)^n}{n!}, \quad n \geq 0,$$

which can be viewed as an iterated sum extension of the well-known result

$$\sum_{\nu=1}^{\infty} \frac{1}{\nu 2^\nu} = \sum_{\nu=1}^{\infty} \frac{(-1)^{\nu+1}}{\nu} = \log 2,$$

typically obtained by comparing the Maclaurin series for $\log(1 + x)$ when $x = -\frac{1}{2}$ and $x = 1$.

We now prove a few results for unit Euler sums that were left as open conjectures in [5]. It will be convenient to employ the following notation:

$$A_r := \mathrm{Li}_r(\tfrac{1}{2}) = \delta(r) = \sum_{k=1}^{\infty} \frac{1}{2^k k^r}, \quad P_r := \frac{(\log 2)^r}{r!}, \quad Z_r := (-1)^r \zeta(r). \tag{47}$$

Theorem 5 *For all positive integers m,*

$$\mu(\{-1\}^m, 1) = (-1)^{m+1} \sum_{k=0}^{m} A_{k+1} P_{m-k} - Z_{m+1}.$$

Proof. ¿From the case (45) of the Hölder convolution, we have

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

Now multiply both sides by $(-1)^m$ and apply the case (42) of δ-duality. □

Remarks. Theorem 5 appeared as the conjectured formula (67) in [5], and is valid for all nonnegative integers m if the divergent $m = 0$ case is interpreted appropriately. The equivalent generating function identity is

$$\sum_{n=1}^{\infty} x^n \mu(\{-1\}^n, 1) = \int_0^{1/2} \frac{(1-t)^x - 1}{t} dt = \log 2 + \sum_{n=1}^{\infty} \left(\frac{1}{x+n} - \frac{1}{n} \right) - \sum_{n=1}^{\infty} \frac{2^{-(x+n)}}{x+n},$$

correcting the misprinted sign in formula (21) of [5].

The asymmetry which marrs Theorem 5 is recovered in the generalization (9), restated and proved below.

Theorem 6 *For all positive integers m and all nonnegative integers n, we have*

$$\begin{aligned} \mu(\{-1\}^m, 1, \{-1\}^n) &= (-1)^{m+1} \sum_{k=0}^{m} \binom{n+k}{n} A_{k+n+1} P_{m-k} \\ &+ (-1)^{n+1} \sum_{k=0}^{n} \binom{m+k}{m} Z_{k+m+1} P_{n-k}, \end{aligned} \tag{48}$$

where A_r, P_r and Z_r are as in (47).

Proof. Let m be a positive integer, and let n be a nonnegative integer. We have

$$\begin{aligned}
\mu(\{-1\}^m, 1, \{-1\}^n) &= (-1)^{m+n+1} \int_0^1 \omega_{-1}^m \omega_1 \int_0^y \omega_{-1}^n \\
&= (-1)^{m+n+1} \int_0^1 \omega_{-1}^m \omega_1 \int_1^{1-y} \omega_2^n \\
&= (-1)^{m+n+1} \int_0^1 \omega_{-1}^m \omega_1 \int_{1/2}^{(1-y)/2} \omega_1^n \\
&= (-1)^{m+n+1} \int_0^1 \omega_{-1}^m \omega_1 \left(\log(1+y)\right)^n /n!.
\end{aligned}$$

By duality,

$$\begin{aligned}
m!n!\mu(\{-1\}^m, 1, \{-1\}^n) &= m! \int_0^1 \left(-\log(2-y)\right)^n \omega_0 \omega_2^m \\
&= m! \int_0^1 \left(-\log(2-y)\right)^n \omega_0 \int_0^{y/2} \omega_1^m \\
&= \int_0^1 \left(-\log(2-y)\right)^n \left(\log(1-y/2)\right)^m \, dy/y.
\end{aligned}$$

Letting $t = 1 - y/2$ and forming the generating function, it follows that

$$\begin{aligned}
\sum_{m=1}^\infty \sum_{n=0}^\infty x^m y^n \mu(\{-1\}^m, 1, \{-1\}^n) &= \sum_{m=1}^\infty \sum_{n=0}^\infty \frac{x^m}{m!} \frac{y^n}{n!} \int_{1/2}^1 \left(-\log(2t)\right)^n (\log t)^m \frac{dt}{1-t} \\
&= \int_{1/2}^1 \frac{(2t)^{-y}\left(t^x - 1\right)}{1-t} \, dt.
\end{aligned}$$

Expanding $1/(1-t)$ in powers of t and integrating term by term yields

$$\begin{aligned}
&\sum_{m=1}^\infty \sum_{n=0}^\infty x^m y^n \mu(\{-1\}^m, 1, \{-1\}^n) \\
&\quad = 2^{-y} \sum_{k=1}^\infty \left(\frac{1}{k+x-y} - \frac{1}{k-y}\right) - \sum_{k=1}^\infty \frac{2^{-(k+x)}}{k+x-y} + \sum_{k=1}^\infty \frac{2^{-k}}{k-y}. \qquad (49)
\end{aligned}$$

It is now a routine matter to extract the coefficient of $x^m y^n$. For the record, here are the details: Since $m \ge 1$, we may ignore the terms in (49) which are independent of x. Thus

$$\begin{aligned}
\mu(\{-1\}^m, 1, \{-1\}^n) &= [x^m y^n] \left\{ \sum_{k=1}^\infty \frac{2^{-y}}{k(1+(x-y)/k)} - \sum_{k=1}^\infty \frac{2^{-(k+x)}}{k(1+(x-y)/k)} \right\} \\
&= [x^m y^n] \left\{ \sum_{r=0}^\infty \frac{1}{r!}(-y\log 2)^r \sum_{k=1}^\infty \frac{1}{k} \sum_{j=0}^\infty \left(\frac{y-x}{k}\right)^j \right.
\end{aligned}$$

$$
\begin{aligned}
& \quad - \sum_{r=0}^{\infty} \frac{1}{r!}(-x \log 2)^r \sum_{k=1}^{\infty} \frac{2^{-k}}{k} \sum_{j=0}^{\infty} \left(\frac{y-x}{k}\right)^j \Bigg\} \\
= \quad & [x^m y^n] \Bigg\{ \sum_{r=0}^{\infty} (-y)^r P_r \sum_{j=1}^{\infty} (y-x)^j \zeta(j+1) \\
& \qquad - \sum_{r=0}^{\infty} (-x)^r P_r \sum_{j=1}^{\infty} (y-x)^j A_{j+1} \Bigg\}, \qquad (50)
\end{aligned}
$$

where we have interchanged order of summation, and used the definitions (47). The inner sums can start at $j = 1$ since we are not extracting the (divergent) constant term from the generating function. We now extract the coefficient of y^n from the first double sum in (50) and at the same time extract the coefficient of x^m from the second double sum in (50). This yields

$$
\begin{aligned}
\mu(\{-1\}^m, 1, \{-1\}^n) \quad = \quad & [x^m] \sum_{k=0}^{n} (-1)^{n-k} P_{n-k} \sum_{j=1}^{\infty} \binom{j}{k} (-x)^{j-k} \zeta(j+1) \\
- \quad & [y^n] \sum_{k=0}^{m} (-1)^{m-k} P_{m-k} \sum_{j=1}^{\infty} \binom{j}{k} y^{j-k} (-1)^k A_{j+1} \\
= \quad & \sum_{k=0}^{n} (-1)^{n-k} P_{n-k} \binom{m+k}{k} (-1)^m \zeta(m+k+1) \\
- \quad & \sum_{k=0}^{m} (-1)^{m-k} P_{m-k} \binom{n+k}{k} (-1)^k A_{n+k+1} \\
= \quad & (-1)^{m+1} \sum_{k=0}^{m} \binom{n+k}{n} A_{k+n+1} P_{m-k} \\
+ \quad & (-1)^{n+1} \sum_{k=0}^{n} \binom{m+k}{m} Z_{k+m+1} P_{n-k},
\end{aligned}
$$

as required. □

Remarks. Theorem 6 is an extension of conjectured formula (68) of [5], and is valid for all nonnegative integers m and n if the divergent $m = 0$ case is interpreted appropriately.

9 Other Integral Transformations

In Section 6, we proved the duality principle for multidimensional polylogarithms by using the integral transformation $y \mapsto 1 - x$. Similarly, in this section we prove more theorems about mutidimensional polylogarithms by using suitable transformations of variables in their integral representations.

Theorem 7 *Let n be a positive integer. Let $b_1, \ldots, b_k$ be arbitrary complex numbers, and let $s_1, \ldots, s_k$ be positive integers. Then*

$$\lambda\binom{s_1, s_2, \ldots, s_k}{b_1^n, b_2^n, \ldots, b_k^n} = n^{s-k} \sum \lambda\binom{s_1, \ldots, s_k}{\varepsilon_1 b_1, \ldots, \varepsilon_k b_k},$$

where the sum is over all n^k cyclotomic sequences

$$\varepsilon_1, \ldots, \varepsilon_k \in \left\{1, e^{2\pi i/n}, e^{4\pi i/n}, \ldots, e^{2\pi i(n-1)/n}\right\},$$

and, as usual, $s := s_1 + s_2 + \cdots + s_k$.

Proof. Write the left-hand side as an iterated integral as in (24):

$$L := \lambda\binom{s_1, s_2, \ldots, s_k}{b_1^n, b_2^n, \ldots, b_k^n} = (-1)^k \int_0^1 \prod_{j=1}^{k} \omega_0^{s_j-1} \omega(b_j^n).$$

Now let $y = x^n$ at each level of integration. This sends ω_0 to $n\omega_0$ and, by partial fractions,

$$\omega(b^n) \mapsto \sum_{r=0}^{n-1} \omega\left(be^{2\pi ir/n}\right).$$

The change of variable gives

$$L = (-1)^k \int_0^1 \prod_{j=1}^{k} (n\omega_0)^{s_j-1} \sum_{r=0}^{n-1} \omega\left(b_j e^{2\pi ir/n}\right).$$

Now carefully expand the noncommutative product and reinterpret each resulting iterated integral as a λ-function to complete the proof. □

Example. When $n = 2$ and $k = 1$, Theorem 7 asserts that

$$\zeta(s) = 2^{s-1} \sum_{n=1}^{\infty} \frac{1 + (-1)^n}{n^s}.$$

Thus, Theorem 7 can be viewed as a cyclotomic extension of the well-known "sum over signs" formula for the alternating zeta function:

$$\sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^s} = (1 - 2^{1-s})\zeta(s), \quad \Re(s) > 0.$$

Next we prove two broad generalizations of formulae (24), (26) and (28) of [5]. By a pair of **Cat** operators we mean nested concatenation (similarly as two $\sum$ signs mean nested summation).

Theorem 8 *Let $s_1, s_2, \ldots, s_k$ be nonnegative integers. Then*

$$\lambda\left(\begin{array}{cccc} 1+s_k, & 1+s_{k-1}, & \ldots, & 1+s_1 \\ -1, & -1, & \ldots, & -1 \end{array}\right) = \sum \mu\left(\operatorname*{\mathbf{Cat}}_{j=1}^{k}\{-1\}\operatorname*{\mathbf{Cat}}_{i=1}^{s_j}\{\varepsilon_{i,j}\}\right)\prod_{j=1}^{k}\prod_{i=1}^{s_j}\varepsilon_{i,j}$$

where the sum is over all $2^{s_1+s_2+\cdots+s_k}$ sequences of signs $(\varepsilon_{i,j})$, with each $\varepsilon_{i,j} \in \{1,-1\}$ for all $1 \le i \le s_j$, $1 \le j \le k$, and **Cat** *denotes string concatenation.*

Proof. Let

$$L := \lambda\left(\begin{array}{cccc} 1+s_k, & 1+s_{k-1}, & \ldots, & 1+s_1 \\ -1, & -1, & \ldots, & -1 \end{array}\right) = (-1)^k \int_0^1 \prod_{j=k}^{1} \omega_0^{s_j}\omega_{-1}.$$

Now let us use duality, and then we let $y = 2t/(1+t)$ at each level of integration. We get

$$L = (-1)^k \int_0^1 \prod_{j=1}^{k} \omega_{-1}(\omega_{-1}-\omega_1)^{s_j}.$$

Now let us carefully expand the noncommutative product. We get

$$L = (-1)^k \sum (-1)^{\#\varepsilon_{i,j}=1} \int_0^1 \prod_{j=1}^{k} \omega_{-1} \prod_{i=1}^{s_j} \omega(\varepsilon_{i,j}),$$

where the sum is over all sign choices $\varepsilon_{i,j} \in \{1,-1\}$, $1 \le i \le s_j$, $1 \le j \le k$, and where by $\#\varepsilon_{i,j} = a$ we mean the cardinality of the set $\{(i,j) \mid \varepsilon_{i,j} = a\}$.

Let us now interpret the interated integtrals as λ-functions. In this case, they are all unit Euler μ-sums, as we defined in (8). Thus,

$$L = (-1)^k \sum (-1)^{\#\varepsilon_{i,j}=1}(-1)^{k+s}\mu\left(\operatorname*{\mathbf{Cat}}_{j=1}^{k}\{-1\}\operatorname*{\mathbf{Cat}}_{i=1}^{s_j}\{\varepsilon_{i,j}\}\right),$$

where, as usual, $s := s_1 + s_2 + \cdots + s_k$. Now if r of the $\varepsilon_{i,j}$ equal $+1$, then $s - r$ of them equal -1. Hence,

$$L = \sum (-1)^{\#\varepsilon_{i,j}=-1}\mu\left(\operatorname*{\mathbf{Cat}}_{j=1}^{k}\{-1\}\operatorname*{\mathbf{Cat}}_{i=1}^{s_j}\{\varepsilon_{i,j}\}\right).$$

Finally, $(-1)^{\#\varepsilon_{i,j}=-1}$ is the same as the product over all the signs $\varepsilon_{i,j}$, and this latter observation completes the proof of Theorem 8. □

Theorem 8 generalizes several identities conjectured in [5]. For example, we get the conjecture (28) of [5] if we put $s_{n+1} = m$, $s_n = s_{n-1} = ... = s_1 = 0$ in Theorem 8. Furthermore, (24) of [5] is the case $s_{m+n+1} = s_{m+n} = ... = s_{n+2} = 0$, $s_{n+1} = 1$, $s_n = s_{n-1} = ... = s_1 = 0$, and (26) of [5] is a special case of Theorem 8 as well.

Thus *every* multidimensional polylogarithm with all alternations (or, equivalently, every Euler sum with first position alternating and all the others non-alternating) is a signed sum over unit Euler sums. The representation of the sign coefficients used in Theorem 8 is much simpler than the cumbersome form of (28) in [5].

Below we present a dual to Theorem 8, which gives *any* unit Euler μ-value in terms of λ-values with all alternations (equivalently, Euler sums with only first position alternating):

Theorem 9 *Let $s_1, s_2, ..., s_k$ be nonnegative integers. Then*

$$\mu\Big(\mathop{\mathbf{Cat}}_{j=0}^{k-1}\{-1\}\{1\}^{s_{k-j}}\Big) = \sum \lambda\Big(\mathop{\mathbf{Cat}}_{j=1}^{k}\mathop{\mathbf{Cat}}_{i=1}^{q_j}\{t_{i,j}-\}\Big)$$

where the sum is over all $2^{s_1+s_2+\cdots+s_k}$ positive integer compositions

$$t_{1,j} + t_{2,j} + ... + t_{q_j,j} = s_j + 1, \qquad 1 \le q_j \le s_j + 1, \quad 1 \le j \le k.$$

Proof. Let

$$M := \mu\Big(\mathop{\mathbf{Cat}}_{j=0}^{k-1}\{-1\}\{1\}^{s_{k-j}}\Big) = (-1)^k \delta\Big(\mathop{\mathbf{Cat}}_{j=1}^{k}\{1+s_j\}\Big) = \int_0^1 \prod_{j=1}^{k} \omega_0^{s_j}\omega_2.$$

Again, let us make the change of variable $y = 2t/(1+t)$ at each level. Then

$$M = \int_0^1 \prod_{j=1}^{k} (\omega_0 - \omega_{-1})^{s_j}(-\omega_{-1}).$$

Again, let us carefully expand the noncommutative product. We get

$$M = \sum (-1)^{\#\varepsilon_{i,j}=-1} \int_0^1 \prod_{j=1}^{k}\left[\prod_{i=1}^{s_j}\omega(\varepsilon_{i,j})\right](-\omega_{-1}),$$

where this time, the sum is over all $\varepsilon_{i,j} \in \{0,-1\}$ with $1 \le i \le s_j$, $1 \le j \le k$.

Note that each ω_{-1} in the integrand contributes -1 to the sign and $+1$ to the depth. Since

$$(-1)^{\text{depth}} \int_0^1 \text{weight-length string} = \lambda(\text{depth-length string}),$$

it follows that M is a sum of λ-values with all $+1$ coefficients. That is,

$$M = \sum \lambda \binom{\vec{t}_1, \ldots, \vec{t}_k}{-1, \ldots, -1},$$

where the sum is over all vectors

$$\vec{t}_j = (t_{1,j}, \ldots, t_{q_j,j}), \qquad 1 \le q_j \le 1 + s_j,$$

and such that

$$\sum_{i=1}^{q_j} t_{i,j} = 1 + s_j, \qquad 1 \le j \le k.$$

In other words, the sum is over all 2^s independent positive integer compositions (in the technical sense of combinatorics) of the numbers $1 + s_j$, $1 \le j \le k$. □

10 Landen's Cousins

Landen's beautiful formulae (see the list (61) below) evidently exhaust the set of polylog evaluations at weight two, depth one in terms of elementary functions [36] (p. 7). In a similar vein, we present here some lovely "weight=depth=2" evaluations, which appear to belong to the same family as Landen's (cf. Coxeter's "ladders" [14] for an alternative extension.)

Theorem 10 *We have the 10 evaluations*

$$\sum_{m=1}^{\infty} \frac{1}{m} \left(\frac{1-\sqrt{5}}{2}\right)^m \sum_{k=1}^{m-1} \frac{1}{k} \left(\frac{3-\sqrt{5}}{2}\right)^k$$
$$= \frac{1}{2} \log^2 \left(\frac{\sqrt{5}-1}{2}\right) + \log\left(\frac{\sqrt{5}-1}{2}\right) \log\left(\frac{\sqrt{5}+1}{2}\right) + \frac{\pi^2}{60}, \tag{51}$$

$$\sum_{m=1}^{\infty} \frac{1}{m} \left(\frac{1-\sqrt{5}}{4}\right)^m \sum_{k=1}^{m-1} \frac{1}{k} \left(\frac{1-\sqrt{5}}{2}\right)^k$$
$$= \frac{1}{2}(\log 2)^2 - \log^2 \left(\frac{\sqrt{5}-1}{2}\right) + \log\left(\frac{\sqrt{5}+1}{2}\right) \log\left(\frac{\sqrt{5}+3}{4}\right) - \frac{\pi^2}{60}, \tag{52}$$

$$\sum_{m=1}^{\infty} \frac{1}{m} \left(\frac{1-\sqrt{5}}{2}\right)^m \sum_{k=1}^{m-1} \frac{1}{k} \left(\frac{1-\sqrt{5}}{2}\right)^k = \log^2\left(\frac{1+\sqrt{5}}{2}\right) - \frac{\pi^2}{30}, \tag{53}$$

$$\sum_{m=1}^{\infty} \frac{1}{m} \left(\frac{3-\sqrt{5}}{2}\right)^m \sum_{k=1}^{m-1} \frac{1}{k2^k}$$

$$= -\frac{1}{2}\log^2\left(\frac{\sqrt{5}-1}{2}\right) - (\log 2)\log\left(\frac{\sqrt{5}-1}{2}\right) - \frac{\pi^2}{60}, \tag{54}$$

$$\sum_{m=1}^{\infty}\frac{(-1)^m}{m}\sum_{k=1}^{m-1}\frac{(-1)^k}{k} = \frac{1}{2}(\log 2)^2 - \frac{\pi^2}{12}, \tag{55}$$

$$\sum_{m=1}^{\infty}\frac{1}{m}\left(\frac{1-\sqrt{5}}{2}\right)^m\sum_{k=1}^{m-1}\frac{(-1)^k}{k}\left(\frac{1+\sqrt{5}}{2}\right)^k$$

$$= \log\left(\frac{\sqrt{5}+3}{2}\right)\log\left(\frac{\sqrt{5}+1}{2}\right) - \log^2\left(\frac{\sqrt{5}-1}{2}\right) - \frac{\pi^2}{15}, \tag{56}$$

$$\sum_{m=1}^{\infty}\frac{1}{m}\left(\frac{3-\sqrt{5}}{4}\right)^m\sum_{k=1}^{m-1}\frac{(-1)^k}{k}\left(\frac{1+\sqrt{5}}{2}\right)^k$$

$$= \frac{1}{2}(\log 2)^2 - \log^2\left(\frac{\sqrt{5}-1}{2}\right) + \log\left(\frac{\sqrt{5}+3}{2}\right)\log\left(\frac{\sqrt{5}+1}{4}\right) + \frac{\pi^2}{60}, \tag{57}$$

$$\sum_{m=1}^{\infty}\frac{(2-\sqrt{5})^m}{m}\sum_{k=1}^{m-1}\frac{(-1)^k}{k}$$

$$= (\log 2)\log(\sqrt{5}-1) + \log^2\left(\frac{\sqrt{5}-1}{2}\right) - \frac{1}{2}(\log 2)^2 - \frac{\pi^2}{60}, \tag{58}$$

$$\sum_{m=1}^{\infty}\frac{(\sqrt{5}-2)^m}{m}\sum_{k=1}^{m-1}\frac{(-1)^k}{k}$$

$$= \log^2\left(\frac{\sqrt{5}-1}{2}\right) + (\log 2)\log(3-\sqrt{5}) - \frac{1}{2}(\log 2)^2 + \frac{\pi^2}{60}, \tag{59}$$

$$\sum_{m=1}^{\infty}\frac{1}{m}\left(\frac{3-\sqrt{5}}{2}\right)^m\sum_{k=1}^{m-1}\frac{(-1)^k}{k}\left(\frac{1+\sqrt{5}}{2}\right)^k$$

$$= \log\left(\frac{\sqrt{5}-1}{2}\right)\log\left(\frac{\sqrt{5}+3}{2}\right) + \frac{\pi^2}{30}. \tag{60}$$

Proof. We require the following

Proposition 1

$$\sum_{m=1}^{\infty}\frac{(-1)^{m+1}x^m}{m}\sum_{k=1}^{m-1}\frac{(-1)^{k+1}y^k}{k} = \log(1+x)\log(1+y) - \mathrm{Li}_2(A) + \mathrm{Li}_2(B),$$

where $A := (1+x)y/(1+y)$ *and* $B := y/(1+y)$*.*

Now recall [36] the following exhaustive list of dilogarithm evaluations due to Landen:

$$\mathrm{Li}_2(0) = 0,$$

$$
\begin{aligned}
\mathrm{Li}_2(1) &= \frac{\pi^2}{6}, \\
\mathrm{Li}_2(-1) &= -\frac{\pi^2}{12}, \\
\mathrm{Li}_2\left(\frac{1}{2}\right) &= \frac{\pi^2}{12} - \frac{1}{2}(\log 2)^2, \\
\mathrm{Li}_2\left(\frac{\sqrt{5}-1}{2}\right) &= \frac{\pi^2}{10} - \log^2\left(\frac{\sqrt{5}-1}{2}\right), \\
\mathrm{Li}_2\left(\frac{1-\sqrt{5}}{2}\right) &= \frac{1}{2}\log^2\left(\frac{\sqrt{5}-1}{2}\right) - \frac{\pi^2}{15}, \\
\mathrm{Li}_2\left(\frac{3-\sqrt{5}}{2}\right) &= \frac{\pi^2}{15} - \log^2\left(\frac{\sqrt{5}-1}{2}\right).
\end{aligned}
\tag{61}
$$

It was a simple matter to program Maple to run through Landen's list (61), thus producing all values of x and y for which both A and B have dilogarithm evaluations and for which the double series converges. The 10 evaluations of Theorem 10 resulted. It now remains only to establish Proposition 1.

Proof of Proposition 1. Interchanging order of summation, we have

$$
\begin{aligned}
\sum_{m=1}^{\infty} \frac{(-1)^m x^m}{m} \sum_{k=1}^{m-1} \frac{(-1)^k y^k}{k} &= \sum_{k=1}^{\infty} \frac{(-1)^k y^k}{k} \sum_{m=k+1}^{\infty} \frac{(-1)^m x^m}{m} \\
&= \sum_{k=1}^{\infty} \frac{(-1)^k y^k}{k} \sum_{m=k+1}^{\infty} (-1)^m \int_0^x t^{m-1}\, dt \\
&= \sum_{k=1}^{\infty} \frac{(-1)^k y^k}{k} \int_0^x \frac{(-1)^{k+1} t^k\, dt}{1+t} \\
&= -\int_0^x \frac{dt}{1+t} \sum_{k=1}^{\infty} \frac{y^k t^k}{k} \\
&= \int_0^x \frac{\log(1-yt)}{1+t}\, dt \\
&= \int_1^{x+1} \frac{\log(1+y-yu)}{u}\, du \\
&= \int_1^{x+1} \frac{\log(1+y)}{u}\, du + \int_1^{x+1} \log\left(1 - \frac{yu}{1+y}\right) \frac{du}{u} \\
&= \log(1+x)\log(1+y) + \int_B^A \frac{\log(1-t)}{t}\, dt \\
&= \log(1+x)\log(1+y) - \mathrm{Li}_2(A) + \mathrm{Li}_2(B),
\end{aligned}
$$

as claimed. □

Remarks. Applying duality to Theorem 10 provides additional insight. We find that formulae (52) and (58) are dual, i.e. equivalent to each other via the duality formula (33). Similarly, formulae (57) and (59) are duals of each other, and hence are equivalent too. Self-dual evaluations are provided by (53) and (60). We have already seen that (55) dualizes to $-\delta(2) = -\mathrm{Li}_2(1/2)$, and similarly, (56) dualizes to

$$-\lambda\left(\frac{2}{\frac{3+\sqrt{5}}{2}}\right) = -\mathrm{Li}_2\left(\frac{3-\sqrt{5}}{2}\right)$$

of Landen's list. Thus, it turns out that only (51) and (54) provide additional evaluations after having taken duality into account. Explicitly they yield

$$\sum_{m=1}^{\infty}\frac{1}{m}\left(\frac{3-\sqrt{5}}{4}\right)^m\sum_{k=1}^{m-1}\frac{2^k}{k} = \frac{1}{2}\log^2\left(\frac{\sqrt{5}-1}{2}\right) + \log\left(\frac{\sqrt{5}-1}{2}\right)\log\left(\frac{\sqrt{5}+1}{2}\right) + \frac{\pi^2}{60},$$

and

$$\sum_{m=1}^{\infty}\frac{(2-\sqrt{5})^m}{m}\sum_{k=1}^{m-1}\frac{1}{k}\left(\frac{3+\sqrt{5}}{2}\right)^k = \frac{1}{2}\log^2\left(\frac{\sqrt{5}-1}{2}\right) + (\log 2)\log\left(\frac{\sqrt{5}-1}{2}\right) + \frac{\pi^2}{60},$$

respectively.

Certainly there must exist analogs to the evaluations of Theorem 10 in the "weight=3" case. Let us just mention the following curiosity:

Lewin ([36], p. 156) gives the evaluation of $\mathrm{Li}_3((3-\sqrt{5})/2)$ where $(3-\sqrt{5})/2 = \theta^2$ for $\theta := 2\sin(\pi/10)$, and also Landen's incorrect (presumably mistyped in Edward's book) evaluation $\mathrm{Li}_3(\theta^2) = \zeta(3)$. Lewin calls this "a little mystery" since nobody has even understood what the supposed equation for $\mathrm{Li}_3(\theta^2)$ intended. In this context it is interesting to note that Theorem 10 states many evaluations with arguments θ and θ^2. Thus, it could be that the "weight=3" analog of Theorem 10 might shed some light on Lewin's "mystery."

11 Functional Equations

One fruitful strategy for proving identities involving special values of polylogarithms is to prove more general (functional, differential) identities and instantiate them at appropriate argument values. In the last two sections of this paper we present examples of such proofs.

Lemma 2 *Let $0 \le x \le 1$ and let*

$$J(x) := \int_0^x \frac{(\log(1-t))^2}{2t}\,dt$$

Then

$$J(-x) = -J(x) + \tfrac{1}{4}J(x^2) + J\left(\frac{2x}{x+1}\right) - \tfrac{1}{8}J\left(\frac{4x}{(x+1)^2}\right). \qquad (62)$$

Proof. If $L(x)$ and $R(x)$ denote the left-hand and the right-hand sides of (62), respectively, then by elementary manipulations (under the assumption $0 < x < 1$) we can show that $dL/dx = dR/dx$. The easy observation $L(0) = R(0) = 0$ then completes the proof. □

Remarks. The identity (62) can be discovered and proved using a computer. Once the "ingredients" (the J-terms) of the identity are chosen, the constant coefficients at them can be determined by evaluating the J-terms at a sufficiently arbitrary value of $x \in]0, 1[$ and using an integer relation algorithm [8]. Once the identity is discovered, the main part of the proof (namely showing that $dL/dx = dR/dx$) can be accomplished in a computer algebra system (e.g., using the `simplify()` command of Maple).

Theorem 11 *We have*

$$\lambda(2-, 1-) = \zeta(2, 1)/8. \qquad (63)$$

Proof. Using notation of Lemma 2 let us observe that

$$J(x) = \sum_{n_1 > n_2 > 0} \frac{x^{n_1}}{n_1^2 n_2}.$$

Plugging in $x = 1$ and applying (62) now completes the proof. □

Remarks. Theorem 11 is the $n = 1$ case of the conjectured identity (23) of [5], namely

$$\lambda(\underbrace{2-, 1-, 2, 1, \ldots}_{2n}) \stackrel{?}{=} 8^{-n}\zeta(\{2, 1\}^n), \qquad (64)$$

for which we have overwhelming numerical evidence. This evidence also suggests that (64) with $n > 1$ seems to be the only case when two Euler sums that do not evaluate (in the sense of the definition in Section 3) have a rational quotient, different from 1. (See also Section 6.2.)

12 Differential Equations and Hypergeometric Series

Here, it is better to work with

$$L(s_1, \ldots, s_k; x) := \lambda_{1/x}(s_1, \ldots, s_k),$$

since then we have

$$\frac{d}{dx}L(s_k,\ldots,s_1;x) = \frac{1}{x}L(-1+s_k,\ldots,s_1;x)$$

if $s_k \geq 2$; while for $s_k = 1$,

$$\frac{d}{dx}L(s_k,\ldots,s_1;x) = \frac{1}{1-x}L(s_{k-1},\ldots,s_1;x).$$

With the initial conditions

$$L(s_k,\ldots,s_1;0) = 0, \quad k \geq 1, \quad \text{and} \quad L(\{\};x) := 1,$$

the differential equations above determine the L-functions uniquely.

12.1 Periodic Polylogarithms

If $\vec{s} := (s_1, s_2, \ldots, s_k)$ and $s := \sum_j s_j$, then every *periodic polylogarithm* $L(\{\vec{s}\}^r)$ has an ordinary generating function

$$L_{\vec{s}}(x,t) := \sum_{r=0}^{\infty} L(\{\vec{s}\}^r;x)t^{rs}$$

which satisfies an algebraic ordinary differential equation in x. In the simplest case, $k = 1$, $\vec{s}$ reduces to the scalar s, and the differential equation for the ordinary generating function is $D_s - t^s = 0$, where

$$D_s := \left((1-x)\frac{d}{dx}\right)^1 \left(x\frac{d}{dx}\right)^{s-1}.$$

The series solution is a generalized hypergeometric function

$$\begin{aligned} L_s(x,t) &= 1 + \sum_{r=1}^{\infty} x^r \frac{t^s}{r^s} \prod_{j=1}^{r-1}\left(1 + \frac{t^s}{j^s}\right) \\ &= {}_sF_{s-1}\left(\left. \begin{array}{c} -\omega t, -\omega^3 t, \ldots, -\omega^{2s-1}t \\ 1, 1, \ldots, 1 \end{array} \right| x \right), \end{aligned}$$

where $\omega = e^{\pi i/s}$, a primitive sth root of -1.

12.2 Proof of Zagier's Conjecture

Let ${}_2F_1(a,b;c;x)$ denote the Gaussian hypergeometric function. Then:

Theorem 12

$$\sum_{n=0}^{\infty} L(\{3,1\}^n; x) t^{4n}$$
$$= {}_2F_1\left(\tfrac{1}{2}t(1+i), -\tfrac{1}{2}t(1+i); 1; x\right) {}_2F_1\left(\tfrac{1}{2}t(1-i), -\tfrac{1}{2}t(1-i); 1; x\right). \quad (65)$$

Proof. Both sides of the putative identity start

$$1 + \frac{t^4}{8}x^2 + \frac{t^4}{18}x^3 + \frac{t^8 + 44t^4}{1536}x^4 + \cdots$$

and are annihilated by the differential operator

$$D_{31} := \left((1-x)\frac{d}{dx}\right)^2 \left(x\frac{d}{dx}\right)^2 - t^4.$$

Once discovered, this can be checked in Mathematica or Maple. □

Corollary 2 (Zagier's Conjecture)[44] *For all nonnegative integers* n,

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

Proof. Gauss's ${}_2F_1$ summation theorem gives

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

Hence, setting $x = 1$ in the generating function (65), we have

$$\begin{aligned}
\sum_{n=0}^{\infty} \zeta(\{3,1\}^n) t^{4n} &= {}_2F_1\left(\tfrac{1}{2}t(1+i), -\tfrac{1}{2}t(1+i); 1; 1\right) {}_2F_1\left(\tfrac{1}{2}t(1-i), -\tfrac{1}{2}t(1-i); 1; 1\right) \\
&= \frac{2}{\pi^2 t^2} \sin(\tfrac{1}{2}(1+i)\pi t) \sin(\tfrac{1}{2}(1-i)\pi t) \\
&= \frac{\cosh(\pi t) - \cos(\pi t)}{\pi^2 t^2} \\
&= \sum_{n=0}^{\infty} \frac{2\pi^{4n} t^{4n}}{(4n+2)!}.
\end{aligned}$$

□

Remark. The proof is Zagier's modification of Broadhurst's, based on the extensive empirical work begun in [5].

12.3 Generalizations of Zagier's Conjecture

In [6] we give an alternative (combinatorial) proof of Zagier's conjecture. This proof is based on combinatorial manipulations of the iterated integral representations of MZVs (see Section 4.2). Using the same technique, we prove in [6] the "Zagier dressed with 2" identity:

$$\sum_{\vec{s}} \zeta(\vec{s}) = \frac{\pi^{4n+2}}{(4n+3)!} \tag{66}$$

where $\vec{s}$ runs over all $2n+1$ possible insertions of the number 2 in the string $\{3,1\}^n$. Still, (66) is just the beginning of a large family of conjectured identities that we discuss in [6].

13 Open Conjectures

The reader has probably noticed that many formulae proved in this paper were conjectured in [5]. For the sake of completeness, we now list formulae from [5] that are still open: (18), (44), (23), (25), (27), (29), (63), and (70)–(74). It is possible that some of these conjectures can be proved using techniques of the present paper.

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