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SPECIAL VALUES OF MULTIPLE POLYLOGARITHMS

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ABSTRACT. Historically, the polylogarithm has attracted specialists and nonspecialists 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 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 an intriguing conjecture of Don Zagier.

1. INTRODUCTION

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

$$l\binom{s_1,\dots,s_k}{b_1,\dots,b_k} := \sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^{k} b_j^{-\nu_j}\left(\sum_{i=j}^{k}\nu_i\right)^{-s_j}, \tag{1.1}$$

and which we shall refer to as *multiple polylogarithms*. When $k = 0$, we define $l(\{\}) := 1$, where $\{\}$ denotes the empty string. When $k = 1$, note that

$$l\binom{s}{b} = \sum_{\nu=1}^{\infty} \frac{1}{\nu^s b^\nu} = \mathrm{Li}_s\left(\frac{1}{b}\right) \tag{1.2}$$

is the usual polylogarithm [49], [50] when s is a positive integer and $|b| \ge 1$. Of course, the polylogarithm (1.2) reduces to the Riemann zeta function [26], [43], [65]

$$\zeta(s) = \sum_{\nu=1}^{\infty} \frac{1}{\nu^s}, \quad \Re(s) > 1, \tag{1.3}$$

when $b = 1$. More generally, for any $k > 0$ the substitution $n_j = \sum_{i=j}^{k} \nu_i$ shows that our multiple polylogarithm (1.1) is related to Goncharov's [35] by the equation

$$\mathrm{Li}_{s_k,\dots,s_1}(x_k,\dots,x_1) = l\binom{s_1,\dots,s_k}{y_1,\dots,y_k}, \quad \text{where} \quad y_j := \prod_{i=1}^{j} x_i^{-1},$$

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and

$$\mathrm{Li}_{s_k,\dots,s_1}(x_k,\dots,x_1) := \sum_{n_1>\cdots>n_k>0} \prod_{j=1}^{k} n_j^{-s_j} {x_j}^{n_j}. \tag{1.4}$$

With each $x_j = 1$, these latter sums (sometimes called *"Euler sums"*), have been studied previously at various levels of generality [2], [6], [7], [9], [13], [14], [15], [16], [31], [38], [39], [42], [51], [59], the case $k = 2$ going back to Euler [27]. Recently, Euler sums have arisen in combinatorics (analysis of quad-trees [30], [46] and of lattice reduction algorithms [23]), knot theory [14], [15], [16], [47], and high-energy particle physics [13] (quantum field theory). There is also quite sophisticated work relating polylogarithms and their generalizations to arithmetic and algebraic geometry, and to algebraic K-theory [4], [17], [18], [33], [34], [35], [66], [67], [68].

In view of these recent applications and the well-known fact that the classical polylogarithm (1.2) often arises in physical problems via the multiple integration of rational forms, one might expect that the more general multiple polylogarithm (1.1) 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 (1.1). On the one hand, the polylogarithm (1.2) has traditionally been studied as a function of b with the positive integer s fixed; while on the other hand, the study of Euler sums has almost exclusively focused on specializations of the nested sum (1.4) in which each $x_j = \pm 1$. 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 are permitted to vary. Indeed, it is our view that it is *impossible* to fully understand the sums (1.2)–(1.4) without viewing them as members of a broader class of multiple polylogarithms.

That said, one might legitimately ask why we chose to adopt the notation (1.1) in favour of Goncharov's (1.4), inasmuch as the latter is a direct generalization of the Li_n notation for the classical polylogarithm. As a matter of fact, the notation (1.4) (with argument list reversed) was our original choice. However, as we reluctantly discovered, it turns out that the notation (1.1), in which the second row of parameters comprises the reciprocated running product of the argument list in (1.4), is more suitable for our purposes here. In particular, our "running product" notation (1.1), in addition to simplifying the iterated integral representation (4.9) (cf. [33] Theorem 16) and the various duality formulae (Section 6; see e.g. equations (6.7) and (6.8)), brings out much more clearly the relationship (Subsection 5.3) between the partition integral (Subection 4.1), in which running products necessarily arise in the integrand; and "stuffles" (Subsections 5.1, 5.2). It seems also that boundary cases of certain formulae for alternating sums must be treated separately unless running product notation is used. Theorem 8.5 with $n = 0$ (Section 8) provides an example of this.

Don Zagier (see e.g. [69]) 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 multiple polylogarithms (1.1) take when the s_j are restricted to the set of positive integers, despite the fact that the sums (1.1) 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 $|b_j| \geq 1$ and $(b_1, s_1) \neq (1, 1)$ to ensure convergence.

Their importance notwithstanding, we feel obliged to confess that our interest in special values extends beyond mere utilitarian concerns. Lewin [49] (p. xi) writes of a "school-boy fascination" with certain numerical results, an attitude which we whole-heartedly 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 [38], [47],

$$\sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^{k} \frac{1}{(\nu_j + \cdots + \nu_k)^2} = \frac{\pi^{2k}}{(2k+1)!}, \qquad 0 \leq k \in \mathbf{Z},$$

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 [7]. The second (see Corollary 1 of Section 8),

$$\begin{aligned}\sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^{k} \frac{(-1)^{\nu_j+1}}{\nu_j + \cdots + \nu_k} &= \sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^{k} \frac{1}{2^{\nu_j}(\nu_j + \cdots + \nu_k)} \\ &= \frac{(\log 2)^k}{k!}, \qquad 0 \leq k \in \mathbf{Z},\end{aligned}$$

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 multiple polylogarithms satisfy. Sections 8 through 11 conclude the paper with proofs of previously conjectured evaluations, including an intriguing conjecture of Zagier [69] and its generalization.

2. Definitions and Additional Examples

A useful specialization of the general multiple polylogarithm (1.1), which is at the same time an extension of the polylogarithm (1.2), is the case in which each $b_j = b$. Under these circumstances, we write

$$\text{(2.1)} \qquad l_b(s_1, \dots, s_k) := l\binom{s_1, \dots, s_k}{b, \dots, b} = \sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^{k} b^{-\nu_j} \left(\sum_{i=j}^{k} \nu_i \right)^{-s_j},$$

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

$$\text{(2.2)} \qquad \zeta := l_1 \quad \text{and} \quad \delta := l_2.$$

The latter δ-function represents an iterated sum extension of the polylogarithm (1.2) with argument one-half, and will play a crucial role in computational issues (Section 7) and "duality" identities such as (1). The former coincides with (1.4) when $k > 0$, each $x_j = 1$, and the order of the argument list is reversed, and hence can be viewed as a multidimensional unsigned Euler sum. We will follow Zagier [69] in referring to these as *"multiple zeta values"* or *"MZVs"* for short. By specifying each $b_j = \pm 1$ in (1.1), *alternating Euler sums* [7] 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 [7] the alternating Euler sums were studied using the notation

$$\zeta(s_1, \ldots, s_k) := \sum_{n_1 > \cdots > n_k > 0} \prod_{j=1}^{k} n_j^{-|s_j|} \sigma_j^{-n_j}$$

where $s_1, \ldots, s_k$ 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,

$$l(\{2-, 1\}^n) := l\begin{pmatrix} 2, 1, \ldots, 2, 1 \\ -1, 1, \ldots, -1, 1 \end{pmatrix} = \sum_{\nu_1, \ldots, \nu_{2n}=1}^{\infty} \prod_{j=1}^{n} \frac{(-1)^{\nu_{2j-1}}}{\left(\sum_{i=2j-1}^{k} \nu_i\right)^2 \left(\sum_{i=2j}^{k} \nu_i\right)}.$$

Unit Euler sums, that is those sums (1.1) in which each $s_j = 1$, are also important enough to be given a distinctive notation. Accordingly, we define

$$\mu(b_1, \ldots, b_k) := l\begin{pmatrix} 1, \ldots, 1 \\ b_1, \ldots, b_k \end{pmatrix} = \sum_{\nu_1, \ldots, \nu_k=1}^{\infty} \prod_{j=1}^{k} b_j^{-\nu_j} \left(\sum_{i=j}^{k} \nu_i\right)^{-1}. \tag{2.3}$$

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 [27], [59], that

$$2\zeta(m, 1) = m\zeta(m+1) - \sum_{k=1}^{m-2} \zeta(m-k)\zeta(k+1), \quad 2 \le m \in \mathbf{Z}.$$

The continued interest in Euler sums is evidenced by the fact that a recent American Mathematical Monthly problem [28] effectively asks for the proof of $\zeta(2, 1) = \zeta(3)$.

Two examples of non-alternating, 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 [69] and proved herein (see Section 11).

Example 2.3.

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

conjectured in [7] and proved by Bowman and Bradley [11].

Example 2.4. An intriguing two-parameter, arbitrary depth evaluation involving alternations, conjectured in [7] and proved herein (see Section 8), is

$$\begin{aligned}\mu(\{-1\}^m,1,\{-1\}^n) &= (-1)^{m+1}\sum_{k=0}^{m}\binom{n+k}{n}A_{k+n+1}P_{m-k}\\ &\quad + (-1)^{n+1}\sum_{k=0}^{n}\binom{m+k}{m}Z_{k+m+1}P_{n-k},\end{aligned}\tag{2.4}$$

where

$$A_r := \mathrm{Li}_r(\tfrac{1}{2}) = \delta(r) = \sum_{k=1}^{\infty}\frac{1}{2^k k^r},\quad P_r := \frac{(\log 2)^r}{r!},\quad Z_r := (-1)^r\zeta(r).\tag{2.5}$$

The formula (2.4) 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

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

Consequently,

$$\begin{aligned}l\binom{s_1,\dots,s_k}{b_1,\dots,b_k} &= \sum_{\nu_1,\dots,\nu_k=1}^{\infty}\prod_{j=1}^{k}b_j^{-\nu_j}D_j\exp\bigg(-u_j\sum_{i=j}^{k}\nu_i\bigg)\\ &= \prod_{j=1}^{k}D_j\sum_{\nu_j=1}^{\infty}b_j^{-\nu_j}\exp\bigg(-\nu_j\sum_{i=1}^{j}u_i\bigg)\\ &= \prod_{j=1}^{k}D_j\bigg\{\frac{1}{b_j\exp\Big(\sum_{i=1}^{j}u_i\Big)-1}\bigg\}.\end{aligned}\tag{2.6}$$

In particular, (2.6) implies

$$l\binom{0,\dots,0}{b_1,\dots,b_k} = \prod_{j=1}^{k}\frac{1}{b_j-1}.\tag{2.7}$$

Despite its utter simplicity, (2.7) points the way to deeper waters. For example, if we put $b_j = q^{-j}$ for each $j=1,2,\dots,k$ and note that

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

then (2.7) implies the generating function equality

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

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 [32] 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 (2.6) yields the numbers [63], (A000629),

$$\delta(-n) = l_2(-n) = \sum_{k=1}^{\infty} \frac{k^n}{2^k} = \mathrm{Li}_{-n}(\tfrac{1}{2}), \qquad 0 \le n \in \mathbf{Z}, \tag{2.8}$$

which enumerate [45] the combinations of a simplex lock having n buttons, and which satisfy the recurrence

$$\delta(-n) = 1 + \sum_{j=0}^{n-1} \binom{n}{j} \delta(-j), \qquad 1 \le n \in \mathbf{Z}.$$

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 [36], [64] that for $n \ge 1$, $\frac{1}{2}\delta(-n)$ also counts

- the number of ways of writing a sum on n indices;
- the number of functions $f : \{1,2,\ldots,n\} \to \{1,2,\ldots,n\}$ such that if j is in the range of f, then so is each value less than or equal to j;
- the number of asymmetric generalized weak orders on $\{1,2,\ldots,n\}$;
- the number of ordered partitions (preferential arrangements) of $\{1,2,\ldots,n\}$.

The numbers $\frac{1}{2}\delta(-n)$ also arise [24] in connection with certain constants related to the Laurent coefficients of the Riemann zeta function. See [63], (A000670), for additional references.

3. Reductions

Given the multiple polylogarithm (1.1), 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, since 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 evidently 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. For example, proving the irrationality of expressions like $\zeta(5,3)/\zeta(5)\zeta(3)$ or $\zeta(5)/\zeta(2)\zeta(3)$ seems to be impossible with current techniques.

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 $\zeta(s,s)$.

One of us (Broadhurst), using high-precision arithmetic and integer relations finding algorithms, has found many conjectured reductions. One example is

$$\zeta(4,1,3) = -\zeta(5,3) + \tfrac{71}{36}\zeta(8) - \tfrac{5}{2}\zeta(5)\zeta(3) + \tfrac{1}{2}\zeta(3)^2\zeta(2), \tag{3.1}$$

which expresses a multiple zeta value of depth three and weight eight in terms of lower depth MZVs, and which was subsequently proved. Observe that the combined weight of each term in the reduction (3.1) is preserved. The easiest proof of (3.1) uses Minh and Petitot's basis of order eight [55].

Broadhurst also noted that although $\zeta(4,2,4,2)$ is apparently irreducible in terms of lower depth MZVs, we have the conjectured[1] weight-12 reduction

$$\begin{aligned}\zeta(4,2,4,2) \stackrel{?}{=} &-\tfrac{1024}{27}l(9-,3) - \tfrac{267991}{5528}\zeta(12) - \tfrac{1040}{27}\zeta(9,3) - \tfrac{76}{3}\zeta(9)\zeta(3)\\ &- \tfrac{160}{9}\zeta(7)\zeta(5) + 2\zeta(6)\zeta(3)^2 + 14\zeta(5,3)\zeta(4)\\ &+ 70\zeta(5)\zeta(4)\zeta(3) - \tfrac{1}{6}\zeta(3)^4\end{aligned} \tag{3.2}$$

in terms of lower depth MZVs *and* the alternating Euler sum $l(9-,3)$. 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 (3.2), namely $l(9-,3)$, $\zeta(9,3)$, 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 [29], 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 (3.1) and (3.2), 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 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 3.1. *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.

[1] Both sides of (3.2) agree to at least 7900 significant figures.

Remark 3.2. The condition on s_1 and s_k is imposed only to ensure convergence of the requisite sums.

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

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

where the sum is over all $\vec{n} = (n_1, n_2, \dots, n_k) \in A \subseteq N$. 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

$$w\biggl(\bigcap_{j=1}^{k-1} N \setminus P_j\biggr) = \sum_{T\subseteq\{1,2,\dots,k-1\}} (-1)^{|T|}\, w\biggl(\bigcap_{j\in T} P_j\biggr). \tag{3.3}$$

We remark that the term on the right-hand side of (3.3) 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 (3.3) is simply $\zeta(s_1, s_2, \dots, s_k)$. Finally, observe that all terms on the right-hand side of (3.3) have depth strictly less than k—except when $T = \{1, 2, \dots, k-1\}$, which gives

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

This latter observation completes the proof of Theorem 3.1. $\square$

4. Integral Representations

Writing the definition of the gamma function [59] 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

$$\begin{aligned} l\binom{s_1, \dots, s_k}{b_1, \dots, b_k} &= \sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^k b_j^{-\nu_j} \biggl(\sum_{i=j}^k \nu_i\biggr)^{-s_j} \\ &= \sum_{\nu_1=1}^\infty \int_1^\infty \frac{(\log x)^{s_1-1}\, dx}{\Gamma(s_1) b_1^{\nu_1} x^{\nu_1+1}} \sum_{\nu_2,\dots,\nu_k=1}^\infty \prod_{j=2}^k (x b_j)^{-\nu_j} \biggl(\sum_{i=j}^k \nu_i\biggr)^{-s_j} \\ &= \frac{1}{\Gamma(s_1)} \int_1^\infty \frac{(\log x)^{s_1-1}}{x b_1 - 1}\, l\binom{s_2, \dots, s_k}{x b_2, \dots, x b_k} \frac{dx}{x}, \end{aligned} \tag{4.1}$$

a representation vaguely remindful of the integral recurrence for the polylogarithm. Repeated application of (4.1) yields the k-dimensional integral representation

$$l\binom{s_1, \dots, s_k}{b_1, \dots, b_k} = \int_1^\infty \cdots \int_1^\infty \prod_{j=1}^k \frac{(\log x_j)^{s_j-1} dx_j}{\Gamma(s_j)\bigl(b_j \prod_{i=1}^j x_i - 1\bigr) x_j}, \tag{4.2}$$

which generalizes Crandall's integral [20] for $\zeta(s_1, \dots, s_k)$. An equivalent formulation of (4.2) is

$$l\binom{s_1, \dots, s_k}{b_1, \dots, b_k} = \int_0^\infty \cdots \int_0^\infty \prod_{j=1}^k \frac{u_j^{s_j - 1}\, du_j}{\Gamma(s_j)(b_j \exp\left(\sum_{i=1}^j u_i\right) - 1)}, \tag{4.3}$$

the integral transforms in (4.3) replacing the derivatives in (2.6).

Although *depth-dimensional integrals* such as (4.2) and (4.3) 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 (4.2), at the expense of increasing the number of integrations. At the extreme, the representation (4.2) is replaced by a *weight-dimensional integral* of a rational function.

4.1. **The Partition Integral.** We begin with the parameters in (1.1). Let $R_1, R_2, \dots, R_n$ be a (disjoint) set partition of $\{1, 2, \dots, k\}$. Put

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

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

$$\begin{aligned} l\binom{r_1, \dots, r_n}{d_1, \dots, d_n} &= \sum_{\nu_1, \dots, \nu_n = 1}^\infty \prod_{m=1}^n d_m^{-\nu_m} \left(\sum_{j=m}^n \nu_j\right)^{-r_m} \\ &= \sum_{\nu_1, \dots, \nu_n = 1}^\infty \prod_{m=1}^n d_m^{-\nu_m} \prod_{i \in R_m} \left(\sum_{j=m}^n \nu_j\right)^{-s_i} \\ &= \sum_{\nu_1, \dots, \nu_n = 1}^\infty \prod_{m=1}^n d_m^{-\nu_m} \int_1^\infty \cdots \int_1^\infty \prod_{i \in R_m} \frac{(\log x_i)^{s_i - 1}\, dx_i}{\Gamma(s_i) x_i^{1 + \nu_m + \cdots + \nu_n}}. \end{aligned}$$

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

$$\begin{aligned} l\binom{r_1, \dots, r_n}{d_1, \dots, d_n} &= \int_1^\infty \cdots \int_1^\infty \left\{ \sum_{\nu_1, \dots, \nu_n = 1}^\infty \prod_{m=1}^n d_m^{-\nu_m} \prod_{j=1}^m \prod_{i \in R_j} x_i^{-\nu_m} \right\} \\ &\quad \times \prod_{j=1}^k \frac{(\log x_j)^{s_j - 1}\, dx_j}{\Gamma(s_j)\, x_j} \\ &= \int_1^\infty \cdots \int_1^\infty \left\{ \prod_{m=1}^n \left(d_m \prod_{j=1}^m \prod_{i \in R_j} x_i - 1 \right)^{-1} \right\} \\ &\quad \times \prod_{j=1}^k \frac{(\log x_j)^{s_j - 1}\, dx_j}{\Gamma(s_j)\, x_j}, \end{aligned} \tag{4.4}$$

on summing the n geometric series.

Example 4.1. Taking $n = k$, we have $R_m = \{m\}$, and $r_m = s_m$ for all $1 \le m \le n$. In this case, (4.4) reduces to the depth-dimensional integral representation (4.2).

Example 4.2. 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 (4.4) yields the seemingly wasteful k-dimensional integral

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

for a polylogarithm of depth one.

Example 4.3. Let $s_j = 1$ for each $1 \le j \le k$, $r_0 = 0$ and let $r_1, r_2, \ldots, r_n$ be arbitrary positive integers with $\sum_{m=1}^{n} r_m = k$. For $1 \le m \le n$ define

$$R_m := \bigcup_{j=1}^{r_m} \left\{ j + \sum_{i=1}^{m-1} r_i \right\}.$$

In this case, (4.4) yields a weight-dimensional integral of a rational function in k variables:

$$l\binom{r_1, \ldots, r_n}{d_1, \ldots, d_n} = \int_1^\infty \cdots \int_1^\infty \left\{ \prod_{m=1}^{n} \left(d_m \prod_{i=1}^{u_m} x_i - 1 \right)^{-1} \right\} \prod_{j=1}^{u_n} \frac{dx_j}{x_j}, \tag{4.5}$$

where $u_m = \sum_{i=1}^{m} r_i$. An interesting specialization of (4.5) 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 above, to use more integrations than are required, nevertheless such a technique allows an easy comparison of multiple polylogarithms having a common weight but possessing widely differing depths. For example, from the four equations

$$\begin{aligned}
l\binom{s+t}{ab} &= \frac{1}{\Gamma(s)\Gamma(t)} \int_1^\infty \int_1^\infty \frac{(\log x)^{s-1} (\log y)^{t-1}\, dx\, dy}{(abxy-1)xy}, \\
l\binom{s, t}{a, ab} &= \frac{1}{\Gamma(s)\Gamma(t)} \int_1^\infty \int_1^\infty \frac{(\log x)^{s-1} (\log y)^{t-1}\, dx\, dy}{(ax-1)(abxy-1)xy}, \\
l\binom{t, s}{b, ab} &= \frac{1}{\Gamma(s)\Gamma(t)} \int_1^\infty \int_1^\infty \frac{(\log x)^{s-1} (\log y)^{t-1}\, dx\, dy}{(by-1)(abxy-1)xy}, \\
l\binom{s}{a} l\binom{t}{b} &= \frac{1}{\Gamma(s)\Gamma(t)} \int_1^\infty \int_1^\infty \frac{(\log x)^{s-1} (\log y)^{t-1}\, dx\, dy}{(ax-1)(by-1)xy},
\end{aligned} \tag{4.6}$$

and the rational function identity

$$\frac{1}{(ax-1)(by-1)} = \frac{1}{abxy-1} \left(\frac{1}{ax-1} + \frac{1}{by-1} + 1 \right), \tag{4.7}$$

the "stuffle" identity (see Section 5.1)

$$l\binom{s}{a} l\binom{t}{b} = l\binom{s, t}{a, ab} + l\binom{t, s}{b, ab} + l\binom{s+t}{ab} \tag{4.8}$$

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 the depth-dimensional integral representation (4.2) 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 [44] 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

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

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

$$b^m m^{-s} = \int_0^b \omega_0^{s-1} y^{m-1}\, dy, \qquad 1 \le m \in \mathbf{Z},$$

one derives from (1.1) that

$$\begin{aligned} l\binom{s_1, \ldots, s_k}{b_1, \ldots, b_k} &= \sum_{\nu_1, \ldots, \nu_k = 1}^{\infty} \prod_{j=1}^k b_j^{-\nu_j} \int_0^{y_{j-1}} \omega_0^{s_j - 1} y_j^{\nu_j - 1}\, dy_j, \quad y_0 := 1\\ &= \prod_{j=1}^k \int_0^{y_{j-1}} \omega_0^{s_j-1} \frac{b_j^{-1}\, dy_j}{1 - b_j^{-1} y_j}\\ &= (-1)^k \int_0^1 \prod_{j=1}^k \omega_0^{s_j-1} \omega(b_j). \end{aligned} \tag{4.9}$$

Letting $s := s_1 + s_2 + \cdots + s_k$ denote the weight, one observes that the representation (4.9) 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:

$$l_q\binom{s_1, \ldots, s_k}{b_1, \ldots, b_k} := l\binom{s_1, \ldots, s_k}{qb_1, \ldots, qb_k} = (-1)^k \int_0^{1/q} \prod_{j=1}^k \omega_0^{s_j-1} \omega(b_j) \tag{4.10}$$

for any real number $q \neq 0$.

Having seen that every multiple polylogarithm can be represented (4.9) by a weight-dimensional iterated integral, it is natural to ask whether the converse holds. In fact, any convergent iterated integral of the form

$$\int_0^1 \prod_{r=1}^s \omega_{\alpha(r)} \tag{4.11}$$

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

$$\int_0^1 \prod_{j=1}^{k} \omega_0^{s_j-1}\omega(b_j) = (-1)^k l\binom{s_1,\dots,s_k}{b_1,\dots,b_k}, \tag{4.12}$$

where

$$0 \neq b_j = \alpha\biggl(\sum_{i=1}^{j} s_i\biggr). \tag{4.13}$$

We remark that the iterated integral representation (4.9) and the weight-dimensional non-iterated integral representation (4.5) of Example 4.3 are equivalent under the change of variable $x_j = y_{j-1}/y_j$, $y_0 := 1$, $j = 1, 2, \dots, s$. In fact, every integral representation of Section 4.1 has a corresponding iterated integral representation under the aforementioned transformation. For example, the depth-dimensional integral (4.2) becomes

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

The explicit observation that MZVs are values of iterated integrals is apparently due to Maxim Kontsevich [69]. Less formally, such representations go as far back as Euler.

5. Shuffles and Stuffles

Although it is natural to study multiple 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 $\vec{s} = (s_1, \dots, s_k)$ and $\vec{t} = (t_1, \dots, t_r)$, we define the set stuffle$(\vec{s}, \vec{t})$ as the smallest set of strings over the alphabet

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

satisfying

- $(s_1, \dots, s_k, t_1, \dots, t_r) \in$ stuffle$(\vec{s}, \vec{t})$.
- 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 $\vec{a} = (a_1, \dots, a_k)$ and $\vec{b} = (b_1, \dots, b_r)$ be two strings of the same length as $\vec{s}$ and $\vec{t}$, respectively. We now define

$$ST := ST\binom{\vec{s}, \vec{t}}{\vec{a}, \vec{b}} \tag{5.1}$$

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

- h is the number of components of $\vec{u}$,
- $c_0 := a_0 := b_0 := 1$,

- 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 l-functions. Consider

$$l\binom{\vec{s}}{\vec{a}} l\binom{\vec{t}}{\vec{b}\ \vec{t}} = \left\{ \sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^{k} a_A j^{-\nu_j} \left(\sum_{i=j}^{k} \nu_i \right)^{-s_j} \right\} \times \left\{ \sum_{\xi_1,\dots,\xi_r=1}^{\infty} \prod_{j=1}^{r} b_j^{-\xi_j} \left(\sum_{i=j}^{r} \xi_i \right)^{-t_j} \right\}.$$

If we put

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

then it follows that

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

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

$$l\binom{\vec{s}}{\vec{a}} l\binom{\vec{t}}{\vec{b}} = \sum l\binom{\vec{u}}{\vec{c}}, \tag{5.2}$$

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 5.1.

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

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 (4.8) was seen to arise from a corresponding rational function identity (4.7) and certain partition integral representations (4.6). This is by no means an isolated phenomenon. In fact, we shall show that *every* stuffle identity is a consequence of the partition integral (4.4) applied to a corresponding rational function identity.

Theorem 5.2. *Every stuffle identity is equivalent to a rational function identity, via the partition integral.*

Before proving Theorem 5.2, we define a class of rational functions, and prove they satisfy a certain rational function identity. Let $\vec{s} = (s_1, \dots, s_k)$ and $\vec{t} = (t_1, \dots, t_r)$ be vectors of positive integers, and let $\vec{\alpha} = (\alpha_1, \dots, \alpha_k)$ and $\vec{\beta} = (\beta_1, \dots, \beta_r)$ be vectors of real numbers. As in (5.1), put

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

and define

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

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

$$f(\gamma_1, \dots, \gamma_h) := \prod_{j=1}^{h} (\gamma_j - 1)^{-1}. \tag{5.3}$$

Then we have the following lemma.

Lemma 5.3. *Let f be defined as in* (5.3). *Then*

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

Proof of Lemma 5.3. Apply (5.2) with $\vec{a} = \vec{\alpha}$ and $\vec{b} = \vec{\beta}$. In view of (2.7), the lemma follows on taking $\vec{s}$ and $\vec{t}$ to be zero vectors of the appropriate lengths. ☐

Proof of Theorem 5.2. Let $\vec{s}$, $\vec{t}$, $\vec{a}$, and $\vec{b}$ be as in (5.2). 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 5.3 and the partition integral representation (4.4) to the depth-dimensional integral (4.2) yields

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

as required. □

5.4. **The Shuffle Algebra.** As opposed to depth-length shuffles, or stuffles, which arise from the definition (1.1) in terms of sums, the iterated integral representation (4.9) gives rise to what are called "*weight-length shuffles*", or simply "shuffles". Weight-length shuffles take the form

$$\int_0^1 \Omega_1\Omega_2\cdots\Omega_n \int_0^1 \Omega_{n+1}\Omega_{n+2}\cdots\Omega_{n+m} = \sum \int_0^1 \Omega_{\sigma(1)}\Omega_{\sigma(2)}\cdots\Omega_{\sigma(n+m)}, \tag{5.4}$$

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.

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

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 multiple polylogarithms comprising the product.

Though it may appear that the shuffles form a rather trivial class of identities satisfied by iterated integrals, it is worth mentioning that the second proof of Zagier's conjecture (see Corollary 2 of Section 11.2) uses little more than the combinatorial properties of shuffles [8]. In addition, both shuffles and stuffles have featured in the investigations of other authors in related contexts [39], [40], [41], [52], [53], [54], [55], [56], [57], [58], [61].

6. Duality

In [38], 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 [69]) follows readily from the iterated integral representation. In [12], 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 multiple polylogarithms, and in this more general setting, has far-reaching implications.

6.1. **Duality for Multidimensional Polylogarithms.**

We begin with the iterated integral representation (4.9) 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

$$l\binom{s_1, \ldots, s_k}{b_1, \ldots, b_k} = (-1)^{s+k} \int_0^1 \prod_{j=k}^{1} \omega(1-b_j)\omega_1^{s_j-1}, \tag{6.1}$$

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

Example 6.1. Using (1.1), (4.9), and (6.1), we have

$$l\binom{2,1}{1,-1} = \int_0^1 \omega(0)\,\omega(1)\,\omega(-1) = -\int_0^1 \omega(2)\,\omega(0)\,\omega(1) = -l\binom{1,2}{2,1},$$

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 $b_1 = b_2 = \cdots = b_k = b$, the two dual iterated integral representations (4.9) and (6.1) simplify as follows:

$$l_b(s_1, \ldots, s_k) = (-1)^k \int_0^1 \prod_{j=1}^{k} \omega_0^{s_j-1}\omega(b) = (-1)^{s+k} \int_0^1 \prod_{j=k}^{1} \omega(1-b)\omega_1^{s_j-1}. \tag{6.2}$$

A somewhat more symmetric version of (6.2) is

$$
\begin{aligned}
(-1)^m l_b(s_1+2,\{1\}^{r_1},\dots,s_m+2,\{1\}^{r_m}) &= (-1)^r \int_0^1 \prod_{j=1}^{m} \omega_0^{s_j+1}\omega_b^{r_j+1} \\
&= (-1)^s \int_0^1 \prod_{j=m}^{1} \omega_{1-b}^{r_j+1}\omega_1^{s_j+1}, \qquad (6.3)
\end{aligned}
$$

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 (6.3), we deduce the *MZV duality formula* (cf. [44], p. 483)

$$
\zeta(s_1+2,\{1\}^{r_1},\dots,s_m+2,\{1\}^{r_m}) = \zeta(r_m+2,\{1\}^{s_m},\dots,r_1+2,\{1\}^{s_1}) \qquad (6.4)
$$

for multidimensional unsigned Euler sums, i.e. multiple zeta values (MZVs) .

Example 6.2. MZV duality (6.4) 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 [60] a beautiful extension of MZV duality (6.4) is given, which also subsumes the so-called sum formula

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

conjectured independently by C. Moen [38] and M. Schmidt [51], and subsequently proved by A. Granville [37]. We refer the reader to Dr. Ohno's article 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 ones completely reduce, i.e. evaluate entirely in terms of (depth-one) Riemann zeta functions.

Example 6.3. The following self-dual evaluation, previously conjectured by Don Zagier [69],

$$
\zeta(\{3,1\}^n) = 4^{-n}\zeta(\{4\}^n) = \frac{2\pi^{4n}}{(4n+2)!}, \qquad 0 \le n \in \mathbf{Z},
$$

is proved herein (see Section 11).

Example 6.4. The evaluation

$$
\begin{aligned}
\zeta(2,\{1,3\}^n) = 4^{-n} \sum_{k=0}^{n} (-1)^k \zeta(\{4\}^{n-k}) \Big\{ & (4k+1)\zeta(4k+2) \\
& - 4\sum_{j=1}^{k} \zeta(4j-1)\zeta(4k-4j+3) \Big\}, \qquad 0 \le n \in \mathbf{Z},
\end{aligned}
$$

conjectured in [7] and recently proved by Bowman and Bradley [11] is also self-dual.

Example 6.5. The self-dual two-parameter generalization of Example 6.3

$$\zeta(\{2\}^m, \{3, \{2\}^m, 1, \{2\}^m\}^n) \stackrel{?}{=} \frac{2(m+1)\pi^{4(m+1)n+2m}}{(2(m+1)(2n+1))!}, \qquad 0 \le m, n \in \mathbf{Z},$$

remains to be proved.

We conclude this section with the following result, since the special case $p = 1$ has some bearing on the MZV duality formula (6.4).

Theorem 6.6. *Let $|p| \ge 1$. The double generating function equality*

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

holds.

Proof. By definition (2.1) of l_p,

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

as claimed. ∎

Remarks 6.7. In [7] it was noted that the $p = 1$ case of Theorem 8.1 is equivalent to the $m = 1$ case of MZV duality (6.4) via the invariance of

$$\begin{aligned}
{}_2F_1\left(\begin{array}{c} y, -x \\ 1-x \end{array} \middle| \, 1 \right) &= \frac{\Gamma(1-x)\Gamma(1-y)}{\Gamma(1-x-y)} \\
&= \exp\left\{ \sum_{k=2}^{\infty} \left(x^k + y^k - (x+y)^k\right) \frac{\zeta(k)}{k} \right\}
\end{aligned} \tag{6.5}$$

with respect to the interchange of x and y. However, it appears that this observation can be traced back to Drinfeld [25]. 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 ([44], p. 468). In our notation, this is essentially the statement that $\zeta(m+2, \{1\}^n) = \zeta(n+2, \{1\}^m)$.

Note that Theorem 8.1 in conjunction with (6.5) 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); taking the coefficient of $x^{m-1}y^3$ provides a much simpler derivation of Markett's formula [51] for $\zeta(m,1,1)$, $m \ge 2$. Thus, the complete reducibility of $\zeta(m+2,\{1\}^n)$ is a simple consequence of the instance (6.5) of Gauss's ${}_2F_1$ hypergeometric summation theorem [1], [3], [62]. Wenchang Chu [19] has elaborated on this idea, applying additional hypergeometric summation theorems to evaluate a wide variety of depth-2 sums, including nonlinear (cf. [31]) sums.

It would be interesting to know if there is a generating function formulation of MZV duality at full strength (6.4). 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 (2.2) as the nested sum extension of the polylogarithm at one-half:

$$\delta(s_1,\dots,s_k) := l\binom{s_1,\dots,s_k}{2,\dots,2} = \sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^{k} 2^{-\nu_j}\left(\sum_{i=j}^{k}\nu_i\right)^{-s_j}. \tag{6.6}$$

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 (2.3) 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 (6.3), we deduce the "delta-to-unit-mu" duality formula

$$\begin{aligned}\delta(s_1+2,\{1\}^{r_1},\dots,s_m+2,\{1\}^{r_m})\\ = (-1)^{r+m}\mu(\{-1\}^{r_m+1},\{1\}^{s_m+1},\dots,\{-1\}^{r_1+1},\{1\}^{s_1+1}).\end{aligned} \tag{6.7}$$

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 (6.2):

$$\delta(s_1,\dots,s_k) = (-1)^k\mu(-1,\{1\}^{s_k-1},\dots,-1,\{1\}^{s_1-1}). \tag{6.8}$$

Example 6.8.

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

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

$$\delta(n+1) = \sum_{\nu=1}^{\infty}\frac{1}{\nu^{n+1}2^{\nu}} = \mathrm{Li}_{n+1}(\tfrac{1}{2}) = -\mu(-1,\{1\}^n). \tag{6.9}$$

Example 6.9. For all nonnegative integers n,

$$\delta(\{1\}^n) = (-1)^n\mu(\{-1\}^n) = (\log 2)^n/n!, \tag{6.10}$$

$$\delta(2,\{1\}^n) = (-1)^{n+1}\mu(\{-1\}^{n+1},1), \tag{6.11}$$

and more generally,

$$\delta(\{1\}^m,2,\{1\}^n) = (-1)^{m+n+1}\mu(\{-1\}^{n+1},1,\{-1\}^m), \qquad 0 \le m,n \in \mathbf{Z}.$$

Example 6.10.

$$\delta(1, n+1) = \mu(-1, \{1\}^n, -1), \qquad 0 \le n \in \mathbf{Z},$$

and in particular, remembering (2.5), (2.8), (6.9) that $\delta(r) = \mathrm{Li}_r(\frac{1}{2})$, we have

$$\begin{aligned}\delta(1,0) &= 1 - \log 2 = 1 - \delta(1),\\ \delta(1,2) &= \tfrac{5}{7}\delta(2)\delta(1) - \tfrac{2}{7}\delta(3) + \tfrac{5}{21}\delta^3(1).\end{aligned}$$

Integer relation searches (see [10] or [7] for details) have failed to find a similar formula for $\delta(1,4)$. However,

$$2\delta(1, 2n-1) = \sum_{j=1}^{2n-1} (-1)^{j+1}\delta(j)\delta(2n-j), \qquad 1 \le n \in \mathbf{Z}.$$

Also,

$$\delta(1, -n) = \sum_{\nu=0}^{n} \binom{n}{\nu} \frac{B_{n-\nu}\delta(-\nu)}{\nu+1}, \qquad 1 \le n \in \mathbf{Z},$$

where the $\delta(-\nu)$ are the simplex lock numbers (2.8) and the B_ν are the Bernoulli numbers [1]. More generally, if n_1 is a positive integer and $n_2, n_3, \dots, n_r$ are all nonnegative integers, then

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

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

Richard Crandall [21] (see also [22]) describes a practical method for fast evaluation of MZVs. Here, we develop an entirely different approach which is based on the fact that any multiple polylogarithm can be expressed as a convolution of rapidly convergent multiple polylogarithms. We have used such representations to compute otherwise slowly convergent alternating Euler sums and (unsigned) MZVs to precisions in the thousands of digits. Lest this strike the reader as perhaps an excessive exercise in recreational computation, consider that many of our results were discovered via exhaustive numerical searches [7] for which even hundreds of digits of precision were insufficient, depending on the type of relation sought [10].

A publicly available implementation of our technique is briefly described in Section 7.2. There are also interesting theoretical considerations which we have only begun to explore. See equations (7.3)–(7.5) below for a taste of what is possible.

7.1. **Derivation and Examples.** We have seen how multiple 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 (4.9) 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 (4.9) and define

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

Then

$$\begin{aligned} l\binom{s_1, \dots, s_k}{b_1, \dots, b_k} &= (-1)^k \int_0^1 \prod_{r=1}^{s} \omega(\alpha_r) \\ &= \sum_{r=0}^{s} (-1)^{r+k} \Big\{ \int_0^{1/q} \prod_{j=r}^{1} \omega(1-\alpha_j) \Big\} \Big\{ \int_0^{1/p} \prod_{j=r+1}^{s} \omega(\alpha_j) \Big\}. \end{aligned} \tag{7.1}$$

Thus, by means of (4.11), (4.12), and (4.13), we have expressed the general multiple polylogarithm as a convolution of l_p with l_q for any p, q such that the Hölder condition $1/p + 1/q = 1$ is satisfied. For this reason, we refer to (7.1) as the *Hölder convolution.* Note that the Hölder convolution generalizes duality (6.1) for multiple polylogarithms, as can be seen by letting p tend to infinity so that (4.10) $l_p \to 0$, and $q \to 1$.

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

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

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

$$\begin{aligned} \vec{a}_j &:= \operatorname*{\mathbf{Cat}}_{i=j}^{m} \{s_i + 2, \{1\}^{r_i}\} = \{s_j + 2, \{1\}^{r_j}, \dots, s_m + 2, \{1\}^{r_m}\}, \\ \vec{b}_j &:= \operatorname*{\mathbf{Cat}}_{i=j}^{1} \{r_i + 2, \{1\}^{s_i}\} = \{r_j + 2, \{1\}^{s_j}, \dots, r_1 + 2, \{1\}^{s_1}\}, \end{aligned}$$

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

$$\begin{aligned} \zeta(\vec{a}_m) = \sum_{j=1}^{m} \Bigg\{ &\sum_{t=0}^{s_j+1} l_p(s_j + 2 - t, \{1\}^{r_j}, \vec{a}_{j+1}) l_q(\{1\}^t, \vec{b}_{j-1}) \\ &+ \sum_{\nu=1}^{r_j} l_p(\{1\}^{\nu}, \vec{a}_{j+1}) l_q(r_j + 2 - \nu, \{1\}^{s_j}, \vec{b}_{j-1}) \Bigg\} + l_q(\vec{b}_m) \\ = \zeta(\vec{b}_m). \end{aligned} \tag{7.2}$$

Of course, $\vec{a}_m$ and $\vec{b}_m$ are the dual strings in the MZV duality formula (6.4). Since the sums l_p converge geometrically, whereas MZV sums converge only polynomially, (7.2) provides an excellent method of computing general MZVs to high precision with the optimal parameter choice $p = q = 2$. For rapid computation of general multiple polylogarithms, it is simplest to use the Hölder convolution (7.1) directly, translating the iterated integrals into geometrically convergent sums on a case by case basis, using (4.9).

Alternating Example.

$$
\begin{aligned}
l(2,1-) &= \int_0^1 \omega(0)\omega(1)\omega(-1) \\
&= \int_0^{1/p} \omega(0)\omega(1)\omega(-1) - \int_0^{1/q} \omega(1) \int_0^{1/p} \omega(1)\omega(-1) \\
&\quad + \int_0^{1/q} \omega(0)\omega(1) \int_0^{1/p} \omega(-1) - \int_0^{1/q} \omega(2)\omega(0)\omega(1) \\
&= l_p(2,1-) + l_p(1,1-)l_q(1) + l_p(1-)l_q(2) - l_q\binom{1,2}{2,1} \\
&= -l\binom{1,2}{2,1}.
\end{aligned}
$$

Although we could now work out the explicit form of the analogue to (7.2) 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 (7.1) gives new relationships between multiple 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 (5.4) 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,

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

Polylog Example. Applying (7.1) to $\zeta(n+2)$, with $p = q = 2$ provides a lovely closed form for $\delta(2, \{1\}^n)$. Indeed,

$$
\zeta(n+2) = \delta(2, \{1\}^n) + \sum_{r=1}^{n+2} \delta(r)\delta(\{1\}^{n+2-r}). \tag{7.3}
$$

The desired closed form follows after rearranging the previous equation (7.3) and applying the definition (6.6) and the result (6.10) in the form $\delta(r) = \mathrm{Li}_r(\frac{1}{2})$ and $\delta(\{1\}^r) = (\log 2)^r/r!$, respectively.

Example 7.1. Putting $n = 1$ in (7.3) gives [5]

$$\zeta(3) = \sum_{n=1}^{\infty} \frac{1}{n^3} = \frac{1}{12}\pi^2 \log(2) + \sum_{n=1}^{\infty} \frac{1}{2^n n^2} \sum_{j=1}^{n} \frac{1}{j}. \tag{7.4}$$

In fact, formula (7.3) is non-trivial even when $n = 0$. Putting $n = 0$ in (7.3) gives the classical evaluation of the dilogarithm at one-half:

$$2\mathrm{Li}_2(\tfrac{1}{2}) = \zeta(2) - (\log 2)^2 \quad \text{i.e.} \quad \sum_{n=1}^{\infty} \frac{1}{2^n n^2} = \tfrac{1}{12}\pi^2 - \tfrac{1}{2}(\log 2)^2. \tag{7.5}$$

Differentiation of (7.1) 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.

7.2. **EZ Face.** A fast program for evaluating MZVs (as well as arithmetic expressions containing them) based on the Hölder convolution formula (7.2) has been developed at the CECM[2], 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/projects/EZFace/`

.

This publicly accessible interface currently allows one to evaluate the sums

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

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

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

for real $p \geq 1$ and positive integers $s_1, \ldots, s_k$. The code for evaluating these sums was written in C, using routines from GMP, the GNU Multiprecision Library[3]. Our implementation permits the precision of the evaluation to be set anywhere between 10 and 100 digits. Progress is currently underway 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 "Using EZ-Face" pages.

In addition to the functions `z` and `zp`, the `lindep` function, based on the LLL algorithm [48] for discovering integer relations [10] satisfied by a vector of real numbers, can be called. 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 $\mathtt{lindep}([x_1, \ldots, x_n])$, where $x_1, \ldots, x_n$ is the vector of values for which the relation is sought. One must ensure that the vector of real numbers is evaluated to sufficient precision to avoid bogus relations and other numerical artifacts. The `lindep` code was written by Michael Monagan and Greg Fee, both of the CECM, and is available on request. Send e-mail to either `monagan@cecm.sfu.ca` or `gjfee@cecm.sfu.ca`.

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

[3] `http://www.swox.com/gmp/`

Below, we give some examples showing how EZ Face may be used. 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.

Example 7.2.
```
Pi^6/z(6)

          945.00000000000000000000000000000000000000000000000000
```

Example 7.3.
```
lindep([z(4,1,3), z(5,3), z(8), z(5)*z(3), z(3)^2*z(2)])

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

Example 7.4.
```
lindep([ z(3), Pi^2*log(2), zp(2,2,1), zp(2,3) ])

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

Example 7.2 is a simple instance of Euler's formula for $\zeta(2n)$. Example 7.3 is the discovery of equation (3.1). Example 7.4 confirms formula (7.4).

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 $p \le -1$ for convergence. Our first result is an easy consequence of the binomial theorem.

Theorem 8.1. *The generating function equality*

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

holds.

Proof. By definition (2.3) 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.

$$\mu(\{p\}^n) = (\log q)^n / n!, \qquad 0 \le n \in \mathbf{Z}.$$

Remarks 8.2. 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 (6.2) takes the particularly appealing form $\mu(\{p\}^n) = (-1)^n \mu(\{1-p\}^n)$ in this context. In particular, $p = -1$ and δ-duality (6.8), (6.10) gives

$$\delta(\{1\}^n) = (-1)^n \mu(\{-1\}^n) = (\log 2)^n/n!, \qquad 0 \le n \in \mathbf{Z},$$

i.e.

$$\begin{aligned}\sum_{\nu_1,\dots,\nu_n=1}^{\infty} \prod_{j=1}^{n} \frac{1}{2^{\nu_j}(\nu_j + \cdots + \nu_n)} &= \sum_{\nu_1,\dots,\nu_n=1}^{\infty} \prod_{j=1}^{n} \frac{(-1)^{\nu_j+1}}{\nu_j + \cdots + \nu_n} \\ &= \frac{(\log 2)^n}{n!}, \qquad 0 \le n \in \mathbf{Z},\end{aligned}$$

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 [7]. It will be convenient to employ the following notation:

$$(8.1) \qquad A_r := \mathrm{Li}_r(\tfrac{1}{2}) = \delta(r) = \sum_{k=1}^{\infty} \frac{1}{2^k k^r}, \quad P_r := \frac{(\log 2)^r}{r!}, \quad Z_r := (-1)^r \zeta(r).$$

Theorem 8.3. *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 (7.3) 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 (6.11) of δ-duality. □

Remarks 8.4. Theorem 8.3 appeared as the conjectured formula (67) in [7], and is valid for all nonnegative integers m if the divergent $m = 0$ case is interpreted appropriately. The equivalent generating function identity is

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

correcting the misprinted sign in formula (21) of [7].

The asymmetry which mars Theorem 8.3 is recovered in the generalization (2.4), restated and proved below.

Theorem 8.5. *For all positive integers m and all nonnegative integers n, we have*

$$\begin{aligned} \mu(\{-1\}^m, 1, \{-1\}^n) &= (-1)^{m+1} \sum_{k=0}^{m} \binom{n+k}{n} A_{k+n+1} P_{m-k} \\ &+ (-1)^{n+1} \sum_{k=0}^{n} \binom{m+k}{m} Z_{k+m+1} P_{n-k}, \end{aligned} \tag{8.2}$$

where A_r, P_r and Z_r are as in (8.1).

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

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

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

$$\begin{aligned} &\sum_{m=1}^{\infty} \sum_{n=0}^{\infty} x^m y^n \mu(\{-1\}^m, 1, \{-1\}^n) \\ &= 2^{-y} \sum_{k=1}^{\infty} \left(\frac{1}{k+x-y} - \frac{1}{k-y} \right) - \sum_{k=1}^{\infty} \frac{2^{-(k+x)}}{k+x-y} + \sum_{k=1}^{\infty} \frac{2^{-k}}{k-y}. \end{aligned} \tag{8.3}$$

Since $m \geq 1$, we may ignore the terms in (8.3) which are independent of x. Thus formally, but with the divergences coming only from the terms independent of x

and hence harmless,

$$\begin{aligned}-2^{-x}\sum_{k=1}^{\infty}\frac{2^{-k}}{k+x-y}+2^{-y}\sum_{k=1}^{\infty}\frac{1}{k+x-y}\\ =-\sum_{r=0}^{\infty}(-x)^r P_r\sum_{h=1}^{\infty}(y-x)^{h-1}A_h-\sum_{r=0}^{\infty}(-y)^r P_r\sum_{h=1}^{\infty}(x-y)^{h-1}Z_h,\end{aligned}$$

where we have used the abbreviations in (8.1). It is now a routine matter to extract the coefficient of $x^m y^n$ to complete the proof. □

Remark 8.6. Theorem 8.5 is an extension of conjectured formula (68) of [7], 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 multiple polylogarithms by using the integral transformation $y \mapsto 1-x$. Similarly, in this section we prove additional results for multiple polylogarithms by using suitable transformations of variables in their integral representations.

Theorem 9.1. *Let n be a positive integer. Let $b_1,\dots,b_k$ be arbitrary complex numbers, and let $s_1,\dots,s_k$ be positive integers. Then*

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

where the sum is over all n^k cyclotomic sequences

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

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

Proof. Write the left-hand side as an iterated integral as in (4.9):

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

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

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

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

Example 9.2. When $n = 2$ and $k = 1$, Theorem 9.1 asserts that

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

Thus, Theorem 9.1 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 [7]. By a pair of **Cat** operators we mean nested concatenation (similarly as two $\sum$ signs mean nested summation).

Theorem 9.3. *Let $s_1, s_2, \ldots, s_k$ be nonnegative integers. Then*

$$l\begin{pmatrix} 1+s_k, & 1+s_{k-1}, & \ldots, & 1+s_1 \\ -1, & -1, & \ldots, & -1 \end{pmatrix} = \sum \mu\Bigg(\mathop{\mathbf{Cat}}_{j=1}^{k} \{-1\} \mathop{\mathbf{Cat}}_{i=1}^{s_j} \{\varepsilon_{i,j}\} \Bigg) \prod_{j=1}^{k} \prod_{i=1}^{s_j} \varepsilon_{i,j}$$

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

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

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 iterated integrals as l-functions. In this case, they are all unit Euler μ-sums, as we defined in (2.3). Thus,

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

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,

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

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 9.3. $\square$

Theorem 9.3 generalizes several identities conjectured in [7]. For example, we get the conjecture (28) of [7] if we put $s_{n+1} = m$, $s_n = s_{n-1} = ... = s_1 = 0$ in Theorem 9.3. Furthermore, (24) of [7] 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 [7] is a special case of Theorem 9.3 as well. Thus *every* multiple 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 9.3 is much simpler than the cumbersome form of (28) in [7].

Below we present a dual to Theorem 9.3, which gives *any* unit Euler μ-value in terms of l-values with all alternations (equivalently, Euler sums with only first position alternating):

Theorem 9.4. *Let $s_1, s_2, ..., s_k$ be nonnegative integers. Then*

$$\mu\left(\operatorname*{\mathbf{Cat}}_{j=0}^{k-1}\{-1\}\{1\}^{s_{k-j}}\right) = \sum l\left(\operatorname*{\mathbf{Cat}}_{j=1}^{k}\operatorname*{\mathbf{Cat}}_{i=1}^{q_j}\{t_{i,j}-\}\right)$$

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

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

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 l-values with all $+1$ coefficients. That is,

$$M = \sum \lambda\begin{pmatrix}\vec{t}_1, \dots, \vec{t}_k\\ -1, \dots, -1\end{pmatrix},$$

where the sum is over all vectors

$$\vec{t_j} = (t_{1,j}, \dots, t_{q_j,j}), \qquad 1 \le q_j \le 1 + s_j,$$

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. 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 10.1. *Let* $0 \le x \le 1$ *and let*

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

Then

$$J(-x) = -J(x) + \tfrac{1}{4}J(x^2) + J\left(\frac{2x}{x+1}\right) - \tfrac{1}{8}J\left(\frac{4x}{(x+1)^2}\right). \tag{10.1}$$

Proof. If $L(x)$ and $R(x)$ denote the left-hand and the right-hand sides of (10.1), 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 10.2. The identity (10.1) 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 [10]. 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 10.3. *We have*

$$l(2-,1-) = \zeta(2,1)/8. \tag{10.2}$$

Proof. Using notation of Lemma 10.1 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 (10.1) now completes the proof. □

Remarks 10.4. Theorem 10.3 is the $n = 1$ case of the conjectured identity (23) of [7], namely

$$l(\underbrace{2-,1-,2,1,\dots}_{2n}) \stackrel{?}{=} 8^{-n}\zeta(\{2,1\}^n), \tag{10.3}$$

for which we have overwhelming numerical evidence. This evidence also suggests that (10.3) 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.)

11. Differential Equations and Hypergeometric Series

Here, it is better to work with

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

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.

11.1. **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

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

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

11.2. **Proof of Zagier's Conjecture.** Let ${}_2F_1(a, b; c; x)$ denote the Gaussian hypergeometric function. Then

Theorem 11.1.

$$\begin{aligned} (11.1) \quad & \sum_{n=0}^{\infty} L(\{3,1\}^n; x) t^{4n} \\ & = {}_2F_1\left(\tfrac{1}{2}t(1+i), -\tfrac{1}{2}t(1+i); 1; x\right) {}_2F_1\left(\tfrac{1}{2}t(1-i), -\tfrac{1}{2}t(1-i); 1; x\right). \end{aligned}$$

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 [69]). *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 (11.1), we have

$$\begin{aligned}
&\sum_{n=0}^{\infty} \zeta(\{3,1\}^n) t^{4n} \\
&= {}_2F_1\left(\tfrac12 t(1+i), -\tfrac12 t(1+i); 1; 1\right) {}_2F_1\left(\tfrac12 t(1-i), -\tfrac12 t(1-i); 1; 1\right) \\
&= \frac{2\sin(\frac12(1+i)\pi t)\sin(\frac12(1-i)\pi t)}{\pi^2 t^2} \\
&= \frac{\cosh(\pi t) - \cos(\pi t)}{\pi^2 t^2} \\
&= \sum_{n=0}^{\infty} \frac{2\pi^{4n} t^{4n}}{(4n+2)!}.
\end{aligned}$$

∎

Remark 11.2. The proof is Zagier's modification of Broadhurst's, based on the extensive empirical work begun in [7].

11.3. **Generalizations of Zagier's Conjecture.** In [8] we give an alternative (combinatorial) proof of Zagier's conjecture, based on combinatorial manipulations of the iterated integral representations of MZVs (see Sections 4.2 and 5.4). Using the same technique, we prove in [8] the "Zagier dressed with 2" identity:

$$\sum_{\vec{s}} \zeta(\vec{s}) = \frac{\pi^{4n+2}}{(4n+3)!} \tag{11.2}$$

where $\vec{s}$ runs over all $2n+1$ possible insertions of the number 2 in the string $\{3,1\}^n$. Still, (11.2) is just the beginning of a large family of conjectured identities that we discuss in [8].

12. Open Conjectures

The reader has probably noticed that many formulae proved in this paper were conjectured in [7]. For the sake of completeness, we now list formulae from [7] that are still open: (18), (23), (25), (27), (29), (44), and (70)–(74). It is possible that some of these conjectures can be proved using techniques of the present paper.

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References

[1] Milton Abramowitz and Irene A. Stegun (eds.) *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables*, Dover, New York, 1972. MR **94b:**00012

[2] David H. Bailey, Jonathan M. Borwein and Roland Girgensohn, *Experimental Evaluation of Euler Sums*, Experiment. Math., **3** (1994), no. 1, 17–30. MR **96e:**11168

[3] Wilfrid Norman Bailey, *Generalized Hypergeometric Series*, Cambridge Tracts in Mathematics and Mathematical Physics, No. 32, Stechert-Hafner, Inc., New York, 1964. MR **32:**2625

[4] A. A. Beilinson, A. B. Goncharov, V. V. Schechtman, and A. N. Varchenko, *Aomoto Dilogarithms, Mixed Hodge Structures and Motivic Cohomology of Pairs of Triangles on the Plane*, the Grothendieck Festschrift, Vol. I, Progr. Math. **86**, Birkhäuser, Boston, (1990), 135–171. MR **92h:**19007

[5] Bruce C. Berndt, *Ramanujan's Notebooks Part I*, Springer-Verlag, New York-Berlin, 1985, p. 258. MR **86c:**01062

[6] David Borwein, Jonathan M. Borwein and Roland Girgensohn, *Explicit Evaluation of Euler Sums*, Proc. Edinburgh Math. Soc., **38** (1995), no. 2, 277–294. MR **96f:**11106

[7] Jonathan M. Borwein, David M. Bradley and David J. Broadhurst, *Evaluations of k-fold Euler/Zagier Sums: A Compendium of Results for Arbitrary k*, Elec. J. Combin., **4** (1997), no. 2, #R5. MR **98b:**11091

[8] Jonathan M. Borwein, David M. Bradley, David J. Broadhurst and Petr Lisoněk, *Combinatorial Aspects of Multiple Zeta Values*, Elec. J. Combin., **5** (1998), no. 1, #R38. MR **99g:**11100.

[9] Jonathan M. Borwein and Roland Girgensohn, *Evaluation of Triple Euler Sums*, Elec. J. Combin., **3** (1996), no. 1, #R23, with an appendix by David J. Broadhurst. MR **97d:**11137

[10] Jonathan M. Borwein and Petr Lisoněk, *Applications of Integer Relation Algorithms*, Discrete Math., Proc. FPSAC'97, special issue, to appear.

[11] Douglas Bowman and David M. Bradley, *Resolution of Some Open Problems Concerning Multiple Zeta Evaluations of Arbitrary Depth*, submitted.

[12] David J. Broadhurst, *Massive 3-loop Feynman Diagrams Reducible to SC* Primitives of Algebras of the Sixth Root of Unity*, Eur. Phys. J. C **8** (1999), 311–333.

[13] ———, *On the Enumeration of Irreducible k-fold Euler Sums and Their Roles in Knot Theory and Field Theory*, to appear in J. Math. Phys.

[14] David J. Broadhurst, John A. Gracey and Dirk Kreimer, *Beyond the Triangle and Uniqueness Relations; Non-Zeta Terms at Large N from Positive Knots*, Zeit. Phys. C, **75** (1997), 559–574. MR **98k:**81178

[15] David J. Broadhurst and Dirk Kreimer, *Knots and Numbers in ϕ^4 Theory to 7 Loops and Beyond*, Internat. J. Modern Phys. C, **6** (1995), no. 4, 519–524. MR **97a:**81143

[16] ———, *Association of Multiple Zeta Values with Positive Knots via Feynman Diagrams up to 9 Loops*, Phys. Lett. B **393** (1997), no. 3-4, 403–412. MR **98g:**11101

[17] Jerzy Browkin, *Conjectures on the Dilogarithm*, K-Theory, **3** (1989), no. 1, 29–56. MR **90m:**11185

[18] ———, *K-Theory, Cyclotomic Equations, and Clausen's Function*, in Structural Properties of Polylogarithms, edited by Leonard Lewin, Amer. Math. Soc. Mathematical Surveys and Monographs **37**, Providence, RI, 1991, 233–273. CMP 92:07

[19] Wenchang Chu, *Hypergeometric series and the Riemann Zeta function*, Acta Arith., **82** (1997), no. 2, 103-118. MR **98m:**11089

[20] Richard E. Crandall, *Topics in Advanced Scientific Computation*, Springer-Verlag, New York; TELOS. The Electronic Library of Science, Santa Clara, CA, 1996. MR **97g:**65005

[21] ———, *Fast Evaluation of Multiple Zeta Sums*, Math. Comp., **67** (1998), no. 223, 1163–1172. MR **98j:**11066

[22] Richard E. Crandall and Joe P. Buhler, *On the evaluation of Euler Sums*, Experiment. Math., **3** (1995), no. 4, 275-285. MR **96e:**11113

[23] Hervé Daudé, Philippe Flajolet and Brigitte Vallée, *An Average-Case Analysis of the Gaussian Algorithm for Lattice Reduction*, Combin. Probab. Comput., **6** (1997), no. 4, 397–433. MR **99a:**65196

[24] Karl Dilcher, *On Generalized Gamma Functions Related to the Laurent Coefficients of the Riemann Zeta Function*, Aequationes Math., **48** (1994), no. 1, 55–85. MR **95h:**11086

[25] V. G. Drinfeld, *On Quasitriangular Quasi-Hopf Algebras and on a Group that is Closely Connected with* Gal($\bar{\mathbf{Q}}/\mathbf{Q}$), (Russian) Algebra i Analiz, **2** (1990), no. 4, 149–181. English translation in Lenningrad Math. J., **2** (1991), no. 4, 829–860. MR **92f:**16047
[26] Harold M. Edwards, *Riemann's Zeta Function*, Pure and Applied Mathematics, Vol. 58, Academic Press, New York-London, 1974. MR **57:**5922
[27] Leonhard Euler, *Meditationes Circa Singulare Serierum Genus*, Novi Comm. Acad. Sci. Petropol., **20** (1775), 140–186, Reprinted in "Opera Omnia", ser. I, **15**, B. G. Teubner, Berlin, 1927, pp. 217–267.
[28] Nicholas R. Farnum, *Problem 10635*, Amer. Math. Monthly, **105** (January 1998), p. 68.
[29] Helaman R. P. Ferguson, David H. Bailey and Steve Arno, *Analysis of PSLQ, An Integer Relation Finding Algorithm*, Math. Comp., **68** (1999), no. 225, 351–369. MR **99c:**11157
[30] Philippe Flajolet, Gilbert Labelle, Louise Laforest and Bruno Salvy, *Hypergeometrics and the Cost Structure of Quadtrees*, Random Structures and Algorithms, **7** (1995), no. 2, 117–144. MR **96m:**68034
[31] Philippe Flajolet and Bruno Salvy, *Euler Sums and Contour Integral Representations*, Experiment. Math., **7** (1998), no. 1, 15–35. MR **99c:**11110
[32] George Gasper and Mizan Rahman, *Basic Hypergeometric Series*, with a forward by Richard Askey. Encyclopedia of Mathematics and Its Applications, **35**, Cambridge University Press, Cambridge, 1990. MR **91d:**33034
[33] Alexander B. Goncharov, *Polylogarithms in Arithmetic and Geometry*, Proceedings of the International Congress of Mathematicians, Vol. 1, 2 (Zürich, 1994), 374–387, Birkhäuser, Basel, 1995. MR **97h:**19010
[34] ———, *The Double Logarithm and Manin's Complex for Modular Curves*, Math. Res. Lett., **4** (1997), no. 5, 617–636. MR **99e:**11086
[35] ———, *Multiple Polylogarithms, Cyclotomy and Modular Complexes*, Math. Res. Lett., **5** (1998), no. 4, 497–516. MR **2000c:**11108
[36] Ian P. Goulden and David M. Jackson, *Combinatorial Enumeration*, with a forward by Gian Carlo-Rota. Wiley-Interscience Series in Discrete Mathematics, John Wiley & Sons, New York, 1983, pp. 186–188, pp. 414–418. MR **84m:**05002
[37] Andrew Granville, *A Decomposition of Riemann's Zeta-Function*, in Analytic Number Theory: London Mathematical Society Lecture Note Series **247**, Y. Motohashi (ed.), Cambridge University Press, 1997, pp. 95–101. MR **2000c:**11134
[38] Michael E. Hoffman, *Multiple Harmonic Series*, Pacific J. Math., **152** (1992), no. 2, 275–290. MR **92i:**11089
[39] ———, *The Algebra of Multiple Harmonic Series*, J. Algebra, **194** (1997), no. 2, 477–495. MR **99e:**11119
[40] ———, *Quasi-Shuffle Products*, J. Alg. Comb., (to appear).
[41] ———, *Algebraic Structures on the Set of Multiple Zeta Values*, preprint.
[42] Michael E. Hoffman and Courtney Moen, *Sums of Triple Harmonic Series*, J. Number Theory, **60** (1996), no. 2, 329–331. MR **98b:**11091
[43] Aleksandar Ivić, *The Riemann Zeta-Function*, (The Theory of the Riemann Zeta-function with Applications), John Wiley and Sons, New York, 1985. MR **87d:**11062
[44] Christian Kassel, *Quantum Groups*, Graduate Texts in Mathematics **155**, Springer-Verlag, New York, 1995. MR **96e:**17041
[45] Joseph D. E. Konhauser, Dan Velleman and Stan Wagon, *Which Way Did The Bicycle Go?*, Mathematical Association of America, 1996, p. 174.
[46] Gilbert Labelle and Louise Laforest, *Combinatorial Variations on Multidimensional Quadtrees*, J. Combin. Theory Ser. A, **69** (1995), no. 1, 1–16. MR **95m:**05018
[47] Tu Quoc Thang Le and Jun Murakami, *Kontsevich's Integral for the Homfly Polynomial and Relations Between Values of Multiple Zeta Functions*, Topology Appl., **62** (1995), no. 2, 193–206. MR **96c:**57017
[48] A. K. Lenstra, H. W. Lenstra Jr. and L. Lovász, *Factoring Polynomials with Rational Coefficients*, Math. Ann., **261** (1982), no. 4, 515–534. MR **84a:**12002
[49] Leonard Lewin, *Polylogarithms and Associated Functions*, Elsevier North Holland, New York-Amsterdam, 1981. MR **83b:**33019
[50] Leonard Lewin (ed.), *Structural Properties of Polylogarithms*, Amer. Math. Soc. Mathematical Surveys and Monographs **37** (1991), Providence, RI. MR **93b:**11158

[51] Clemens Markett, *Triple Sums and the Riemann Zeta Function*. J. Number Theory, **48** (1994), no. 2, 113–132. MR **95f:**11067

[52] Hoang Ngoc Minh, *Summations of Polylogarithms via Evaluation Transform*, Mathematics and Computers in Simulation, **42** (1996), 707–728.

[53] ———, *Fonctions de Dirichlet d'ordre n et de Paramètre t*, Discrete Math., **180** (1998), 221–241.

[54] Hoang Ngoc Minh and Michel Petitot, *Mots de Lyndon: Générateurs de Relations entre les Polylogarithmes de Nielsen*, presented at FPSAC (Formal Power Series and Algebraic Combinatorics), Vienna, July 1997.

[55] ———, *Lyndon words, Polylogarithms and the Riemann ζ Function*, Discrete Math. (to appear).

[56] Hoang Ngoc Minh, Michel Petitot and Joris van der Hoeven, *Shuffle Algebra and Polylogarithms*, in Proc. FPSAC'98, the 10th International Conference on Formal Power Series and Algebraic Combinatorics, Toronto, June 1998.

[57] ———, *L'algèbre des Polylogarithmes par les Séries Génératrices*, presented at FPSAC (Formal Power Series and Algebraic Combinatorics), Barcellona, June 1999.

[58] ———, *Computation of the Monodromy of Generalized Polylogarithms*, preprint.

[59] Niels Nielsen, *Die Gammafunktion*, Chelsea, New York, 1965, pp. 47–49. MR **32:**2622

[60] Yasuo Ohno, *A Generalization of the Duality and Sum Formulas on the Multiple Zeta Values*, J. Number Theory, **74** (1999), 39–43. MR **99k:**11138

[61] Chris Reutenauer, *Free Lie Algebras*, London Math. Soc. Monog. **7** (new series), Clarendon Press, Oxford Sciences Publications, Oxford, 1993. MR **94j:**17002

[62] Lucy Joan Slater, *Generalized Hypergeometric Functions*, Cambridge University Press, Cambridge, 1966. MR **34:**1570

[63] Neil J. A. Sloane, *Online Encyclopedia of Integer Sequences*, http://www.research.att.com/~njas/sequences/.

[64] Richard P. Stanley, *Enumerative Combinatorics*, Vol. I, Wadsworth & Brooks/Cole Mathematical Series, Monterey, California, 1986, p. 146. MR **87j:**05003

[65] Edward Charles Titchmarsh, *The Theory of the Riemann Zeta-function*, (2nd ed.) revised by D. R. Heath-Brown, The Clarendon Press, Oxford University Press, New York, 1986. MR **88c:**11049

[66] Zdzislaw Wojtkowiak, *The Basic Structure of Polylogarithmic Functional Equations*, in Structural Properties of Polylogarithms, edited by Leonard Lewin, Amer. Math. Soc. Mathematical Surveys and Monographs **37**, Providence, RI, 1991, 205–231. CMP 92:07

[67] ———, *Functional Equations of Iterated Integrals with Regular Singularities*, Nagoya Math. J., **142** (1996), 145–159. MR **98b:**14018

[68] ———, *Mixed Hodge Structures and Iterated Integrals I*, June, 1999. [K-theory preprint #351, http://www.math.uiuc.edu/K-theory]

[69] Don Zagier, *Values of Zeta Functions and their Applications*, First European Congress of Mathematics, Vol. II (Paris, 1992), Prog. Math., **120**, Birkhäuser, Basel-Boston, (1994), 497–512. MR **96k:**11110

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