Central Binomial Sums, Multiple Clausen Values, and Zeta Values

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CONTENTS

We find and prove relationships between Riemann zeta values and central binomial sums. We also investigate alternating binomial sums (also called Apéry sums). The study of nonalternating sums leads to an investigation of different types of sums which we call multiple Clausen values. The study of alternating sums leads to a tower of experimental results involving polylogarithms in the golden ratio.

1. INTRODUCTION

We shall begin by studying the *central binomial sum* $S(k)$, given as

$$S(k) := \sum_{n=1}^{\infty} \frac{1}{n^k \binom{2n}{n}}$$

for integer k. A classical evaluation is $S(4) = \frac{17}{36}\zeta(4)$. Using a mixture of integer relation and other computational techniques, we uncover remarkable links to values of multi-dimensional polylogarithms of sixth roots of unity which we call multiple Clausen values. We are thence able to prove some surprising identities — and empirically determine many more. Our experimental *integer relation* tools are described in some detail in [Borwein and Lisoněk 2000].

We shall finish by discussing the corresponding alternating sum:

$$A(k) := \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n^k \binom{2n}{n}}.$$

These are related to *polylogarithmic ladders* in the golden ratio $\frac{1}{2}(\sqrt{5}-1)$. A classical evaluation is

$$A(3) = \tfrac{2}{5}\zeta(3),$$

with its connections to Apéry's proof of the irrationality of $\zeta(3)$; see [Borwein and Borwein 1987], for example.

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2. DEFINITIONS AND PRELIMINARIES

We start with some definitions which for the most part follow [Lewin 1981; Borwein et al. 1997; 1998; 2001]. A useful *multi-dimensional polylogarithm* is defined by

$$\mathrm{Li}_{a_1,\ldots,a_k}(z) := \sum_{n_1>\ldots>n_k>0} \frac{z^{n_1}}{n_1^{a_1}\ldots n_k^{a_k}},$$

with the parameters required to be positive integers. This is a generalization of the familiar polylogarithm $\mathrm{Li}_n(z) := \sum_{k=1}^{\infty} z^k/k^n$. Note that $\mathrm{Li}_n(1) = \zeta(n)$.

We will be most concerned with the value of the multi-dimensional polylogarithm at the sixth root of unity, $\omega := e^{i\pi/3}$. We refer to such a value as a *multiple Clausen value* (MCV) and write

$$\mu(a_1,\ldots,a_k) := \mathrm{Li}_{a_1,\ldots,a_k}(\omega).$$

This MCV is analogous to the multiple zeta value (MZV), at $z = 1$, which has been studied in works such as [Borwein et al. 1997; 1998; 2001]. We might also have viewed these values as generalizations of the *Lerch zeta* function. It transpires to be advantageous to separate the real and imaginary parts of an MCV in a manner that is based on the sum of the arguments. We refer to these parts as *multiple Glaishers* (mgl) and *multiple Clausens* (mcl). They are defined by

$$\begin{aligned}\mathrm{mgl}(a_1,\ldots,a_k) &:= \mathrm{Re}(i^{a_1+\cdots+a_k}\mu(a_1,\ldots,a_k)),\\ \mathrm{mcl}(a_1,\ldots,a_k) &:= \mathrm{Im}(i^{a_1+\cdots+a_k}\mu(a_1,\ldots,a_k)),\end{aligned}$$

and may be written explicitly as multiple sin or cos sums depending on the parity. For example, when $a+b$ is odd,

$$\mathrm{mgl}(a,b) = \pm\sum_{n>m>0} \frac{\sin(n\pi/3)}{n^a m^b},$$

as is the case in Theorem 3.3 below.

As elsewhere, the *weight* of a sum is $\sum_{i=i}^{k} a_i$ while the *depth* k is the number of parameters. This separation corresponds, in the case $k = 1$, to Lewin's [1981] separation of the polylogarithm at complex exponential arguments into Clausen and Glaisher functions.

We record the following differential properties of our multi-dimensional polylogarithm:

$$\frac{d\,\mathrm{Li}_{a_1+2,a_2,\ldots,a_n}(z)}{dz} = \frac{\mathrm{Li}_{a_1+1,\ldots,a_n}(z)}{z}, \tag{2–1}$$

$$\frac{d\,\mathrm{Li}_{1,a_2,\ldots,a_n}(z)}{dz} = \frac{\mathrm{Li}_{a_2,\ldots,a_n}(z)}{1-z}. \tag{2–2}$$

Repeated application of (2–2) yields

$$\mathrm{Li}_{\{1\}^n}(z) = \frac{(-\log(1-z))^n}{n!}, \tag{2–3}$$

where $\{1\}^n$ denotes the string $1,\ldots,1$ with n ones.

We will make use of the *Bernoulli polynomials* later in this paper. Recall that $B_n(x)$ is defined by

$$\frac{te^{xt}}{e^t-1} = \sum_{n=0}^{\infty} B_n(x)\frac{t^n}{n!},$$

and that $B_n(0)$ is called the *n-th Bernoulli number* and is written B_n.

For convenience we choose the following notation for *log-sine integrals*:

$$j(a,b) := \int_0^{\pi/3} \left(\log\left(2\sin\frac{\theta}{2}\right)\right)^a \theta^b d\theta \tag{2–4}$$

and

$$r(a,b) := \frac{i^{b+1}}{a!b!}\int_0^{\pi/3} \left(\log\left(2\sin\frac{\theta}{2}\right)+\frac{i}{2}\left(\theta-\pi\right)\right)^a \theta^b d\theta. \tag{2–5}$$

Finally, a standard result involving the *gamma function* will prove very useful:

$$a^{-n}\Gamma(n) = \int_0^1 y^{a-1}(-\log y)^{n-1}dy.$$

3. NONALTERNATING CENTRAL BINOMIAL SUMS

Our first step is to write $S(k)$ in integral form.

Lemma 3.1. *For all positive integers k,*

$$S(k) = \frac{(-2)^{k-2}}{(k-2)!}\,j(k-2,1).$$

Proof. We employ the gamma function and various standard tricks. First

$$\begin{aligned}S(k) &= \sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}n^k}\\ &= \sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}\Gamma(n)}\int_0^1 (-\log x)^{k-1}x^{n-1}dx;\end{aligned}$$

setting $y^2 = x$ and integrating by parts, this becomes

$$= \sum_{n=1}^{\infty} \frac{1}{\binom{2n}{n}\Gamma(n)} \int_0^1 (-2\log y)^{k-1} y^{2n-2}(2y)\,dy$$

$$= -\sum_{n=1}^{\infty} \frac{(-2)^{k-1}}{\binom{2n}{n}\Gamma(n)} \left(\int_0^1 \frac{y^{2n}}{2n} 2(k-1)\frac{(\log y)^{k-2}}{y} dy\right)$$

$$= \frac{(-2)^{k-1}}{(k-2)!} \int_0^1 \frac{(\log y)^{k-2}}{y} \sum_{n=1}^{\infty} \frac{y^{2n}}{n\binom{2n}{n}} dy.$$

Using [Borwein and Borwein 1987, p. 384] we get

$$S(k) = \frac{(-2)^{k-1}}{(k-2)!} \int_0^1 \frac{(\log y)^{k-2}}{y} \frac{y \arcsin(y/2)}{\sqrt{1-(y/2)^2}} dy$$

$$= \frac{(-2)^{k-2}}{(k-2)!} \int_0^{\pi/3} (\log(2\sin\theta/2))^{k-2} \theta\, d\theta$$

with the change of variables $y = 2\sin\theta/2$. □

Hence to evaluate the sums $S(k)$, it is enough to determine log-sine integrals of the *special* form $j(k,1)$. The key is the following identity:

Lemma 3.2. *For all* $k > 2$,

$$\sum_{r=0}^{k-2} \frac{(-i\pi/3)^r}{r!} \mu(k-r, \{1\}^n)$$
$$= \zeta(k,\{1\}^n) - (-1)^{k+n} r(n+1, k-2). \quad (3\text{–}1)$$

Proof. First note the formal identity

$$\log(1-e^{i\theta}) = \log\left(2\sin\frac{\theta}{2}\right) + \frac{i}{2}(\theta - \pi). \quad (3\text{–}2)$$

We have, by (2–1),

$$\mu(k,\{1\}^n) = \zeta(k,\{1\}^n) + \int_1^{\omega} \frac{\mathrm{Li}_{k-1,\{1\}^n}(z)}{z} dz.$$

We now integrate by parts repeatedly to obtain

$$\mu(k,\{1\}^n) = \zeta(k,\{1\}^n) - \sum_{r=1}^{k-2} \frac{(-1)^r \mu(n-r,\{1\}_k)\log^r\omega}{r!}$$
$$+ \frac{(-1)^{k-2}}{(k-2)!} \int_1^{\omega} \frac{\mathrm{Li}_{\{1\}_{n+1}}(z)\log^{k-2} z}{z} dz.$$

Observe that $\log\omega = i\pi/3$. Let $z = e^{i\theta}$. Then, using (2–3),

$$\mu(k,\{1\}^n) = \zeta(k,\{1\}^n) - \sum_{r=1}^{k-2} \frac{(-i\pi/3)^r \mu(n-r,\{1\}_k)}{r!}$$
$$+ \frac{i(-1)^k}{(k-2)!\,(n+1)!} \int_0^{\pi/3} (-\log(1-e^{i\theta}))^{n+1}(i\theta)^{k-2} d\theta,$$

which gives us the desired result upon application of (3–2). □

Now, note that $r(a,b)$, defined in (2–5), can be expanded out binomially and written as linear rational combination of $j(c,d)$, defined in (2–4), for various c,d, including a nonzero multiple of $j(a,b)$. So we may repeatedly use the above identity to solve for each $j(a,b)$ in terms of multiple Clausen, Glaisher and zeta values — all of the same form $\mathrm{mcl}(n,\{1\}_k)$, $\mathrm{mgl}(n,\{1\}_k)$ and $\zeta(n,\{1\}_k)$.

In particular, for all k, $j(k-2,1)$ and hence $S(k)$ can be written as a linear rational combination of multiple zeta, Clausen and Glaisher values of this form. This method, which we have automated in Reduce and in Maple, recovers all previously known results in a uniform fashion. It does not in general give especially nice looking identities, but we are able to apply some other results about multiple Clausen values derived in the next section to clean things up for small k. After doing this, we obtain the following evaluations of central binomial sums:

Theorem 3.3.

$$S(2) = \tfrac{1}{3}\zeta(2)$$
$$S(3) = -\tfrac{2}{3}\pi\,\mathrm{mcl}(2) - \tfrac{4}{3}\zeta(3)$$
$$S(4) = \tfrac{17}{36}\zeta(4)$$
$$S(5) = 2\pi\,\mathrm{mcl}(4) - \tfrac{19}{3}\zeta(5) + \tfrac{2}{3}\zeta(3)\zeta(2)$$
$$S(6) = -\tfrac{4}{3}\pi\,\mathrm{mgl}(4,1) + \tfrac{3341}{1296}\zeta(6) - \tfrac{4}{3}\zeta(3)^2$$
$$S(7) = -6\pi\,\mathrm{mcl}(6) - \tfrac{493}{24}\zeta(7) + 2\zeta(5)\zeta(2) + \tfrac{17}{18}\zeta(4)\zeta(3)$$
$$S(8) = -4\pi\,\mathrm{mgl}(6,1) + \tfrac{3462601}{233280}\zeta(8) - \tfrac{14}{15}\zeta(5,3)$$
$$- \tfrac{38}{3}\zeta(5)\zeta(3) + \tfrac{2}{3}\zeta(2)\zeta(3)^2.$$

The results for $S(2)$ and $S(4)$ are classical evaluations. That for $S(3)$ seems first to have appeared in print in [Ghusayni 1998]. The others, and the general analysis, are new and it is hoped that they will shed light on odd ζ-values, which remain a source of many unanswered questions. We observe that genuine MCVs, with depth $k > 1$, first occur for $n = 6$ and 8. Moreover, David Bailey and David Broadhurst have explicitly obtained $S(n)$ for $n \le 20$ through a very high level application of integer relation algorithms. The result for $S(20)$ is presented in [Bailey and Broadhurst 2001].

4. MULTIPLE CLAUSEN VALUES

Central binomial sums naturally led us into a study of multiple Clausen values. This study proved to be quite fruitful and we were led to many striking results.

To start with, we quote from [Lewin 1981] some results about depth-one Clausen values:

$$\operatorname{mgl}(n) = \frac{(-1)^{n+1}2^{n-1}\pi^n B_n(\frac{1}{6})}{n!}, \tag{4–1}$$
$$\operatorname{mcl}(2n+1) = \frac{(-1)^n}{2}(1-2^{-2n})(1-3^{-2n})\zeta(2n+1).$$

4A. MCV Duality

In MZV analysis, one of the central results is the now well-known MZV *duality theorem* recapitulated in [Borwein et al. 1997]:

$$\zeta(a_1+2, \{1\}_{b_1}, \dots, a_k+2, \{1\}_{b_k}) = \zeta(b_k+2, \{1\}_{a_k}, \dots b_1+2, \{1\}_{a_1}),$$

For all positive integers $a_1, a_2, \dots, a_n$.

For MCV's, we have found two such duality results, with the first result applying if the first argument of the MCV is one (such sums converge as in the classical Fourier setting) while the second holds if the first argument of the MCV is two or more. The pattern in Theorem 4.2 is somewhat complicated. A prior example may make things clearer.

Example 4.1. $\mu(1,3,1,2) - \mu(1)\,\mu(3,1,2) + \mu(2) \times \mu(2,1,2) - \mu(3)\,\mu(1,1,2) + \mu(1,3)\,\mu(1,2) - \mu(1,1,3) \times \mu(2) + \mu(2,1,3)\,\mu(1) - \mu(1,2,1,3) = 0.$

Each summand differs from its predecessor by subtracting '1' from the first argument of the right MCV and adding '1' to the first argument of the left MCV. In the case where there is a '1' as the first argument of the right MCV, this '1' is dropped and concatenated onto the left MCV.

Theorem 4.2. *For all positive integers $a_1, a_2, \dots, a_n$, we have*

$$\begin{aligned}&\mu(1,a_1,\dots,a_n) - \mu(1)\mu(a_1,\dots,a_n)\\ &+\mu(2)\mu(a_1-1,\dots,a_n) + \dots \pm \mu(a_1)\mu(1,a_2,\dots,a_n)\\ &\mp \mu(1,a_1)\mu(a_2,\dots,a_n) + \dots \pm \mu(1,a_n,\dots,a_1) = 0.\end{aligned}$$

Proof. We prove this by repeated integration by parts. We use the differential properties (2–1) and (2–2) to move weight from one multidimensional polylogarithm to another:

$$\begin{aligned}&\mu(1,a_1,\dots,a_n)\\ &= \int_0^\omega \frac{\operatorname{Li}_{a_1,\dots,a_n}(z)}{1-z}dz\\ &= \big[\operatorname{Li}_1(z)\operatorname{Li}_{a_1,\dots,a_n}(z)\big]_0^\omega - \int_0^\omega \frac{\operatorname{Li}_1(z)\operatorname{Li}_{a_1-1,\dots,a_n}(z)}{z}dz\\ &= \dots = \dots \pm \mu(1,a_n,\dots,a_1).\end{aligned}$$ □

As in other duality results, it is interesting to examine what happens in the self-dual case. Suppose that $(a_1,\dots,a_n) = (a_n,\dots,a_1)$; then, if $a_1+\dots+a_n$ is even, the equation in Theorem 4.2 reduces to $0=0$. If the sum is odd, the same equation shows that $\mu(1,a_1,\dots,a_n)$ reduces to a sum and product of lower weight MCVs.

The pattern in Theorem 4.4 below is more complicated. Hence an example will be even more instructive. The bar denotes complex conjugation.

Example 4.3. $\mu(4,3,1) + \overline{\mu(1)}\,\mu(3,3,1) + \overline{\mu(1,1)} \times \mu(2,3,1) + \overline{\mu(1,1,1)}\,\mu(1,3,1) + \overline{\mu(2,1,1)}\,\mu(3,1) + \overline{\mu(1,2,1,1)}\mu(2,1) + \overline{\mu(1,1,2,1,1)}\mu(1,1) + \overline{\mu(2,1,2,1,1)} \times \mu(1) + \overline{\mu(3,1,2,1,1)} = \zeta(3,1,2,1,1).$

Each summand differs from its predecessor by subtracting '1' from the first argument of the right MCV and concatenating '1' onto the left MCV. In the case where there is a 1 as the first argument of the right MCV, this '1' is dropped and '1' is added to the first argument of the left MCV .

Theorem 4.4 is specialization of the *Hölder convolution* [Borwein et al. 2001, (44)] with $p=\omega$ and $q = 1-\omega = \overline{\omega}$. That paper gives a more formal description of the pattern of summation that we have outlined above.

Theorem 4.4. *For all positive integers $a_1, a_2, \cdots, a_n$,*

$$\begin{aligned}&\mu(a_1+2, \{1\}_{b_1}, \dots, a_k+2, \{1\}_{b_k})\\ &\quad+\overline{\mu(1)}\mu(a_1+1, \{1\}_{b_1}, \dots, a_k+2, \{1\}_{b_k}) + \dots\\ &\quad+\overline{\mu(\{1\}_{a_1+1})}\mu(1, \{1\}_{b_1}, \dots, a_k+2, \{1\}_{b_k})\\ &\quad+\overline{\mu(2, \{1\}_{a_1})}\mu(\{1\}_{b_1}, \dots, a_k+2, \{1\}_{b_k}) + \dots\\ &\quad+\overline{\mu(b_1+2, \{1\}_{a_1})}\mu(a_2+2, \dots, a_k+2, \{1\}_{b_k}) + \dots\\ &\quad+\overline{\mu(b_k+2, \{1\}_{a_k}, \dots, b_1+2, \{1\}_{a_1})}\\ &\qquad= \zeta(b_k+2, \{1\}_{a_k}, \dots, b_1+2, \{1\}_{a_1}).\end{aligned}$$

Proof. As stated above, this follows by Hölder convolution, since $\operatorname{Li}_{\vec{a}}(\overline{\omega}) = \overline{\mu(\vec{a})}$. It can also be proved using a similar integration by parts as above, using the differentiation properties

$$\frac{d\,\mathrm{Li}_{a_1+2,a_2,\dots,a_n}(1-z)}{dz} = -\frac{\mathrm{Li}_{a_1+1,a_2,\dots,a_n}(1-z)}{1-z},$$
$$\frac{d\,\mathrm{Li}_{1,a_2,\dots,a_n}(1-z)}{dz} = -\frac{\mathrm{Li}_{a_2,\dots,a_n}(1-z)}{z}.$$

This identity allows us to move weight from a multi-dimensional polylogarithm at z to one at $1-z$. □

This suggested integration by parts technique also yields a new proof for this type of Hölder convolution. Hence, it provides another proof of MZV duality.

In this case, self-dual strings do not tell us that much. The only thing to note is that all the imaginary terms on left side of the equation in Theorem 4.4 will vanish, since $a\bar{b} + \bar{a}b$ is real. When $k = 1$, the equation simplifies, on using (4–1), to

$$\zeta(a+2,\{1\}_b) + \frac{(-1)^a(i\pi/3)^{a+b+2}}{(a+1)!(b+1)!} = \sum_{r=0}^{a} \frac{(-i\pi/3)^r}{r!}\mu(a+2-r,\{1\}_b) + \sum_{r=0}^{b} \frac{(i\pi/3)^r}{r!}\overline{\mu(b+2-r,\{1\}_a)}. \tag{4–2}$$

We initially derived (4–2) by means of (3–1) and a satisfying identity involving log-sine integrals, which we proved using contour integration:

$$(-1)^{a+b}\zeta(a{+}2,\{1\}_{b-1}) = \frac{(i\pi/3)^{a+1}(-i\pi/3)^b}{(a{+}1)!b!} - \overline{r(a{+}1,b{-}1)} - r(b,a).$$

4B. Special values of MCVs

To illustrate the utility of this last duality result, consider (4–2) when $a = 1$ and $b = 1$. We obtain

$$\zeta(3,1) - 2\,\mathrm{mgl}(3,1) - \frac{2\pi}{3}\,\mathrm{mgl}(2,1) - \frac{\pi^4}{324} = 0.$$

Using MZV analysis [Borwein et al. 2001], we know that $\zeta(3,1) = \pi^4/360$, which is the first case in an infinite series of evaluations in terms of powers of π^4, conjectured by Zagier and proved in [Borwein et al. 1998]. Now from (4–5) below we have

$$\mathrm{mgl}(2,1) = \frac{\pi^3}{324}.$$

This rewards us with

$$\mathrm{mgl}(3,1) = \frac{-23}{19440}\pi^4.$$

Next, we use the duality result to extract some more general evaluations. Let

$$F(x,y) := \sum_{a,b\ge 0} \mu(a{+}2,\{1\}_b)\,x^{a+1}y^{b+1}.$$

According to [Borwein et al. 2001], we know that this generating function is *hypergeometric*:

$$F(x,y) = 1 - {}_2F_1(-x,y;1{-}x;\omega). \tag{4–3}$$

Unfortunately, this is not a very convenient equation for extracting coefficients or proving formulas. To get a more useful representation, we take (4–2), multiply through by $x^{a+1}y^{b+1}$ and sum over all $a, b \ge 0$. This gives

$$e^{-i\pi x/3}F(x,y) + e^{i\pi y/3}\overline{F(y,x)} + (e^{-i\pi x/3}-1)(e^{i\pi y/3}-1) = G(x,y),$$

where

$$G(x,y) := \sum_{a,b\ge 0} \zeta(a+2,\{1\}_b)x^{a+1}y^{b+1}$$

is the generating function for the corresponding multiple zeta values. Now from prior work on MZVs [Borwein et al. 1997] it is known that

$$G(x,y) = 1 - \exp\left(\sum_{k\ge 2} \frac{x^k + y^k - (x+y)^k}{k}\zeta(k)\right).$$

We shall use this generating function identity to obtain more general results about special values of mgl's and mcl's. First we put the last identity in a more symmetric form by letting

$$M(x,y) := F(ix,-iy) = \sum_{a,b\ge 0}(-1)^{b+1}\big(\mathrm{mgl}(a{+}2,\{1\}_b) + i\,\mathrm{mcl}(a{+}2,\{1\}_b)\big)x^{a+1}y^{b+1}.$$

Then

$$e^{\pi x/3}M(x,y) + e^{\pi y/3}\overline{M(y,x)} + (e^{\pi x/3}-1)(e^{\pi y/3}-1) = G(ix,-iy). \tag{4–4}$$

Theorem 4.5. *For nonnegative integers a and b,*

$$\mathrm{mgl}(\{1\}_a,2,\{1\}_b) = (-1)^{a+b+1}\frac{(\pi/3)^{a+b+2}}{2(a+b+2)!}, \tag{4–5}$$

and this value depends only on $a + b$.

Proof. First we show that

$$\operatorname{mgl}(2,\{1\}_b) = (-1)^{b+1}\frac{(\pi/3)^{b+2}}{2(b+2)!}.$$

We give two proofs of this result.

(i) Multiply by y/x in (4–4), and let x go to zero. Set

$$B(y) := \sum_{b=0}^{\infty}(-1)^{b+1}\operatorname{mgl}(2,\{1\}_b)y^{b+2},$$

$$C(y) := \sum_{b=0}^{\infty}(-1)^{b+1}\operatorname{mgl}(b+2)y^{b+2},$$

$$D(y) := \sum_{m=1}^{\infty}(-1)^{2m+m-1}\zeta(2,\{1\}_{2m-2})y^{2m}.$$

Comparing real parts on each side of (4–4) yields

$$B(y) + e^{\pi y/3}C(y) + \frac{\pi y}{3}(e^{\pi y/3}-1) = D(y).$$

The value of $\operatorname{mgl}(n)$ and so of $C(y)$ is given by (4–1), while MZV duality yields $\zeta(2,\{1\}_{2m-2}) = \zeta(2m)$ with its familiar Bernoulli number evaluation. Combining these results and using the generating function for the Bernoulli polynomials, we arrive at

$$B(y) = \frac{e^{\pi y/3}}{2} - \frac{\pi y}{6} - \frac{1}{2},$$

which implies

$$\operatorname{mgl}(2,\{1\}_b) = (-1)^{b+1}\frac{(\pi/3)^{b+2}}{2(b+2)!}.$$

(ii) Alternatively, we start with (4–3). Dividing by x, setting $y = iy$, and letting x go to zero yields

$$-i\sum_{n=1}^{\infty}\frac{(iy)_n\omega^n}{nn!} = \frac{\sum_{b=0}^{\infty}\mu(a{+}2,\{1\}_b)(iy)^{b+2}}{y}.$$

Now we know that

$$\sum_{n=1}^{\infty}\frac{(iy)_n z^{n-1}}{n!} = \frac{(1-z)^{-iy}-1}{z}.$$

Integrate both sides of this expression from 0 to ω along $z = 1+e^{i(\pi-\theta)}$, where $2\pi/3 \le \theta \le \pi$, to obtain

$$\sum_{n=1}^{\infty}\frac{(iy)_n\omega^n}{n\,n!} = -i\int_0^{\pi/3}\frac{(e^{-\theta y}-1)(1-\cos\theta+i\sin\theta)}{2-2\cos\theta}d\theta - i\left(\frac{e^{-\pi y/3}}{y} - \frac{1}{y} + \frac{\pi}{3}\right).$$

This again gives us

$$\operatorname{Im}\left(\sum_{n=1}^{\infty}\frac{(iy)_n\omega^n}{n\,n!}\right) = -\frac{e^{-\pi y/3}+\pi y/3-1}{2y}$$

as required.

Armed with this special case, we now prove the full result for $\operatorname{mgl}(\{1\}_a,2,\{1\}_b)$. We start with a similar integration by parts as for the proof of (3–1). We have

$$\begin{aligned}\mu(\{1\}_b,2,\{1\}_a) &= \int_0^{\omega}\frac{\operatorname{Li}_{\{1\}_{b-1},2,\{1\}_a}(z)}{1-z}\,dz\\ &= \frac{i\pi}{3}\mu(\{1\}_{b-1},2,\{1\}_a) + \cdots\\ &\qquad + (-1)^{b+1}\frac{(i\pi/3)^b}{b!}\mu(2,\{1\}_a)\\ &\qquad + \int_0^{\omega}\frac{(\log(1-z))^b\operatorname{Li}_{\{1\}_{a+1}}(z)}{b!\,z}\,dz\end{aligned}$$

by repeated integration by parts, which in turn is seen to equal

$$\frac{i\pi}{3}\mu(\{1\}_{b-1},2,\{1\}_a)+\cdots+(-1)^{b+1}\frac{(i\pi/3)^b}{b!}\mu(2,\{1\}_a) + (-1)^b\binom{a{+}b{+}1}{b}\mu(2,\{1\}_{a+b})$$

using (2–3).

Now, multiplying through by i^{a+b+2}, extracting real parts and proceeding by induction we find that we must show that

$$\binom{a{+}b{+}2}{0} + \cdots + (-1)^b\binom{a{+}b{+}2}{b} = (-1)^b\binom{a{+}b{+}1}{b}.$$

However,

$$\binom{a{+}b{+}2}{i} = \binom{a{+}b{+}1}{i} + \binom{a{+}b{+}1}{i{-}1},$$

and it is now easily seen that the left side telescopes. □

4C. Additional Evaluations

We can use (4–4) to obtain a clean expression for the alternating sum of all mgl's of the form $\operatorname{mgl}(a,\{1\}_b)$ of fixed weight. Let

$$A(x) := \sum_{n=1}^{\infty}\left(\sum_{m=0}^{n-2}(-1)^{m+1}\operatorname{mgl}(n{+}2{-}m,\{1\}_m)\right)x^n.$$

If we set $x = y$ in(4–4), after some work we obtain

$$A(x) = \frac{1}{2}\left(-\frac{\pi x e^{-\pi x/3}}{\sinh \pi x} - e^{\pi x/3} + 2\right) = \frac{1}{2}\left(-\frac{2\pi x e^{2\pi x/3}}{e^{2\pi x} - 1} - e^{\pi x/3} + 2\right).$$

This leads to

$$\sum_{m=0}^{n-2} (-1)^{m+1} \operatorname{mgl}(n+2-m, \{1\}_m) = \frac{-\pi^n}{2n!}\left(B_n\left(\tfrac{1}{3}\right)2^n + \left(\tfrac{1}{3}\right)^n\right).$$

We note that this equation is equivalent to

$$\operatorname{Re}\big(1 - {}_2\mathrm{F}_1(-ix, -ix; 1-ix; \omega)\big) = \operatorname{Re}\left(\sum_{n=1}^{\infty} \frac{(-ix)(-ix)_n}{n - ix}\omega^n\right) = -\frac{1}{2}\left(\frac{\pi x e^{-\pi x/3}}{\sinh(\pi x)} + e^{\pi x/3} - 2\right),$$

on using the hypergeometric representation of the underlying generating function. We have not managed to prove this by more direct methods.

An unusual-looking class of identities may be extracted from (4–3) on setting $y = 1 - x$. This gives

$$1 - e^{-i\pi x/3} = \sum_{a,b \geq 0} \mu(a+2, \{1\}_b) x^{a+1}(1-x)^{b+1},$$

which — when we extract the coefficients of various powers of x on both sides — gives us curious infinite sums of MCVs of different weight, reminiscent of similar rational ζ-evaluations [Borwein et al. 2000]. For example, extracting the coefficient of x yields

$$\sum_{b=0}^{\infty} \mu(2, \{1\}_b) = \frac{i\pi}{3}.$$

More generally, we obtain

$$\sum_{b=0}^{\infty}\left(\mu(n+1, \{1\}_b) - (b+1)\mu(n, \{1\}_b) + \cdots + (-1)^{n+1}\binom{b+1}{n-1}\mu(2, \{1\}_b)\right) = -\frac{(-i\pi/3)^n}{n!}.$$

5. MCV DIMENSIONAL CONJECTURES

While there do not appear to be many other closed form evaluations, it is apparent that there is still more to be learned by examining all MCVs — and especially their integral representations. This is a subject we have largely ignored in this paper, but which figures large in [Broadhurst 1999], where polylogarithms of the sixth root of unity were studied in the context of integrals arising from quantum field theory.

Experiments using linear relation algorithms suggested that the only MCVs that evaluate to rational multiples of powers of π are those already identified, namely $\operatorname{mgl}(3,1)$ and $\operatorname{mgl}(\{1\}_b, 2, \{1\}_a)$. Moreover we found no other nontrivial reduction of an MCV to a single rational multiple of powers of other MCVs. Nevertheless, our integer relation searches suggested a very simple enumeration of the basis size for MCVs of a given weight.

Consider the set

$$\mathcal{C}(n) := \{\operatorname{mcl}(a_1, \ldots, a_k) : a_1 + \cdots + a_k = n\}$$

of all multiple Clausen values of fixed weight, n. We wish to determine the smallest set of real numbers such that each element of $\mathcal{C}(n)$ can be written as a rational linear combination of elements from this set. This will consist of mcl's of that weight or products of lower weight mcl's, mgl's, MZV's and powers of π. We denote by $I(n)$ the size of the basis for $\mathcal{C}(n)$. Similarly, we denote by $R(n)$ the basis size for multiple Glaisher values of weight n.

Our first conjecture is quite striking:

Conjecture 5.1. *The following* twisted Fibonacci *recursion obtains*:

$$R(n) = R(n-1) + I(n-2),$$
$$I(n) = I(n-1) + R(n-2),$$
$$R(0) = R(1) = 1, \quad I(0) = I(1) = 0.$$

A corollary is that $W(n) := R(n) + I(n)$, the total size of a rational basis for MCV's of weight n, should satisfy

$$W(n) = W(n-1) + W(n-2),$$

which delightfully gives the Fibonacci sequence.

Looking at things more finely, we examined the number $P(n,k)$ of *irreducibles* of weight n and depth k, such that a rational basis at this weight and depth is formed from a minimum number of irreducibles, augmented by products of irreducibles of lesser weight and depth. Again, we are lead to a rather striking conjecture:

Conjecture 5.2. *This weight and depth filtration is generated by*

$$\prod_{n>1,k>0}(1-x^n y^k)^{P(n,k)} = 1-\frac{x^2 y}{1-x}.$$

Both conjectures have been intensively checked by the PSLQ algorithm [Bailey and Broadhurst 2001] for $k \le n \le 7$. They provide compelling evidence that there is a great deal of structure to MCVs. It seems unlikely that they will be proved soon, since they imply, *inter alia*, the irrationality of $\zeta(n)$ for all odd n. The interested reader has online access to some of the code we have used and also an interface for more general integer relation problems; see section on Electronic Availability at the end.

6. APÉRY SUMS AND THE GOLDEN LADDER

By way of comparison we present results for the alternating binomial sums

$$A(k) := \sum_{n>0} \frac{(-1)^{n+1}}{\binom{2n}{n} n^k}.$$

As we now describe, we found that the cases $k = 2$, 3, 4, 5, 6 reduce to classical polylogarithms of powers of

$$\rho := \frac{\sqrt{5}-1}{2},$$

the reciprocal of the golden section. The ladder that generates these results extends up to $\zeta(9)$. Details of *polylogarithmic ladder* techniques are to be found in [Lewin 1991].

The results for $k < 5$ were proved by classical methods (and also obtained by John Zucker, private communication). For $k \ge 5$, we were content to rely on the empirical methods adopted in [Lewin 1991], determining rational coefficients from high precision numerical computations.

• <u>At $k = 2$</u> one easily obtains from Clausen's hypergeometric square [Abramowitz and Stegun 1972; Borwein and Borwein 1987] the result

$$A(2) = 2L^2,$$

where

$$L := \log \rho.$$

Indeed, we found 6 integer relations between $A(2)$, $\zeta(2)$, and the dilogarithms $\{\mathrm{Li}_2(\rho^p) \mid p \in \mathcal{C}\}$, where $\mathcal{C} := \{1, 2, 3, 4, 6, 8, 10, 12, 20, 24\}$, generates the corresponding cyclotomic relations [Lewin 1991].

In general, it is more convenient to work with the set

$$\mathcal{K}_k := \{L_k(\rho^p) \mid p \in \mathcal{C}\}$$

of *Kummer-type polylogarithms*, of the form

$$\begin{aligned} L_k(x) :&= \frac{1}{(k-1)!}\int_0^x \frac{(-\log|y|)^{k-1}dy}{1-y} \\ &= \sum_{r=0}^{k-1} \frac{(-\log|x|)^r}{r!}\,\mathrm{Li}_{k-r}(x) \end{aligned}$$

where as before $\mathrm{Li}_k(x) := \sum_{n>0} x^n/n^k$.

• <u>At $k = 3$</u> one has Apéry's result

$$A(3) = \tfrac{2}{5}\zeta(3).$$

Moreover there are 5 integer relations between $\mathcal{K}_3$, L^3, and $\zeta(3)$.

• <u>At $k = 4$</u> we recently proved a result, using classical polylogarithmic theory, which simplifies to

$$A(4) = 4\tilde{L}_4(\rho) - \tfrac{1}{2}L^4 - 7\zeta(4)$$

where

$$\tilde{L}_k(x) := L_k(x) - L_k(-x) = 2L_k(x) - 2^{1-k}L_k(x^2).$$

In fact, there are 5 integer relations between $\mathcal{K}_4$, L^4, $\zeta(4)$ and $A(4)$. Another simple example is

$$A(4) = \tfrac{16}{9}\tilde{L}_4(\rho^3) - 2L^4 - \tfrac{23}{9}\zeta(4).$$

• <u>At $k = 5$</u> we found four empirical integer relations between $\mathcal{K}_5$, L^5, $\zeta(5)$ and $A(5)$. The simplest result is

$$A(5) = \tfrac{5}{2}L_5(\rho^2) + \tfrac{1}{3}L^5 - 2\zeta(5).$$

More explicitly, with $\rho := (\sqrt{5}-1)/2$, this produces

$$\begin{aligned} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5\binom{2k}{k}} &= 2\zeta(5) - \tfrac{4}{3}\log(\rho)^5 + \tfrac{8}{3}\log(\rho)^3\zeta(2) \\ &\quad + 4\log(\rho)^2\zeta(3) + 80\sum_{n>0}\left(\frac{1}{(2n)^5} - \frac{\log(\rho)}{(2n)^4}\right)\rho^{2n}, \end{aligned}$$

which, along with previous integer relation exclusion bounds (see [Bailey and Borwein 2000; Borwein and Lisoněk 2000], for example), helps explain why no 'simple' evaluation for $A(5)$ such as those for $S(2)$, $A(3)$, and $S(4)$ has ever been found.

• <u>At $k = 6$</u> we found the empirical relation

$$\begin{aligned} &11\left\{A(6) - \tfrac{2}{5}\zeta^2(3)\right\} \\ &\quad = 144\tilde{L}_6(\rho) - \tfrac{64}{9}\tilde{L}_6(\rho^3) + \tfrac{9}{5}L^6 - \tfrac{2434}{9}\zeta(6), \end{aligned}$$

which is the simplest of three integer relations between $\mathcal{K}_6$, L^6, $\zeta(6)$ and the combination $A(6) - \frac{2}{5}\zeta^2(3)$.

• At $k = 7$ there are 2 integer relations between $\mathcal{K}_7$, L^7, and $\zeta(7)$. There is no result for $A(7)$ from this set; presumably $A(7)$ occurs in combination with some other weight-7 irreducible, of which $\zeta^2(3)$ was a harbinger, at $k = 6$.

• At $k = 8$ there is a single integer relation.

• At $k = 9$ the ladder terminates with a single integer relation, namely

$$\begin{aligned}
&2791022262\,\zeta(9)\\
&\quad = 15750\,L_9(\rho^{24}) + 74277\,L_9(\rho^{20}) - 8750000\,L_9(\rho^{12})\\
&\qquad - 19014912\,L_9(\rho^{10}) - 206671500\,L_9(\rho^{8})\\
&\qquad + 1295616000\,L_9(\rho^{6}) - 3180657375\,L_9(\rho^{4})\\
&\qquad + 4907952000\,L_9(\rho^{2}) - 52537600\log^9(\rho).
\end{aligned}$$

This still falls short of the ladder for $\zeta(11)$ found in [Broadhurst 1998]. The current record is set by the ladder for $\zeta(17)$ in [Bailey and Broadhurst 1999], which extends the weight-16 analysis of Henri Cohen, Leonard Lewin and Don Zagier [Cohen et al. 1992], in the number field of the Lehmer polynomial of conjecturally smallest Mahler measure.

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ELECTRONIC AVAILABILITY

See http://www.cecm.sfu.ca/projects/ezface+/ for some of the code we have used in the investigations reported here. A CECM interface for more general integer relation problems is available at http://www.cecm.sfu.ca/projects/IntegerRelations/.

NOTE ADDED IN PROOF

Since this paper was accepted we've learned that E. Remiddi and J. A. M. Vermaseren [2000] studied a cognate class of polylogarithms. Relations like those of Theorem 4.2 are also in their paper.

REFERENCES

[Abramowitz and Stegun 1972] M. Abramowitz and I. A. Stegun (editors), *Handbook of mathematical functions with formulas, graphs, and mathematical tables*, Dover, New York, 1972. Reprinted 1992.

[Bailey and Borwein 2000] D. H. Bailey and J. M. Borwein, "Experimental mathematics: recent developments and future outlook", in *Mathematics unlimited:* 2001 *and beyond*, edited by B. Engquist and W. Schmid, Springer, New York, 2000.

[Bailey and Broadhurst 1999] D. H. Bailey and D. J. Broadhurst, "A seventeenth-order polylogarithm ladder", 1999, http://arxiv.org/abs/math.CA/9906134.

[Bailey and Broadhurst 2001] D. H. Bailey and D. J. Broadhurst, "Parallel integer relation detection: techniques and applications", *Math. Comp.* (2001). See http://arxiv.org/abs/math.NA/9905048.

[Borwein and Borwein 1987] J. M. Borwein and P. B. Borwein, *Pi and the AGM: a study in analytic number theory and computational complexity*, Wiley, New York, 1987. Reprinted 1998.

[Borwein and Lisoněk 2000] J. M. Borwein and P. Lisoněk, "Applications of integer relation algorithms", *Discrete Math.* **217**:1-3 (2000), 65–82.

[Borwein et al. 1997] J. M. Borwein, D. M. Bradley, and D. J. Broadhurst, "Evaluations of k-fold Euler/Zagier sums: a compendium of results for arbitrary k", *Electron. J. Combin.* **4**:2 (1997), RP 5, 21 pp.

[Borwein et al. 1998] J. M. Borwein, D. M. Bradley, D. J. Broadhurst, and P. Lisoněk, "Combinatorial aspects of multiple zeta values", *Electron. J. Combin.* **5**:1 (1998), RP 38, 12 pp.

[Borwein et al. 2000] J. M. Borwein, D. M. Bradley, and R. E. Crandall, "Computational strategies for the Riemann zeta function", *J. Comput. Appl. Math.* **121**:1-2 (2000), 247–296.

[Borwein et al. 2001] J. M. Borwein, D. M. Bradley, D. J. Broadhurst, and P. Lisoněk, "Special values of multidimensional polylogarithms", *Trans. Amer. Math. Soc.* (2001). See http://arxiv.org/abs/math.CA/9910045.

[Broadhurst 1998] D. J. Broadhurst, "Polylogarithmic ladders, hypergeometric series and the ten millionth digits of $\zeta(3)$ and $\zeta(5)$", preprint, 1998. See http://arxiv.org/abs/math.CA/9803067.

[Broadhurst 1999] D. J. Broadhurst, "Massive 3-loop Feynman diagrams reducible to SC* primitives of algebras of the sixth root of unity", *Eur. Phys. J. C Part. Fields* **8**:2 (1999), 313–333.

[Cohen et al. 1992] H. Cohen, L. Lewin, and D. Zagier, "A sixteenth-order polylogarithm ladder", *Experiment. Math.* **1**:1 (1992), 25–34.

[Ghusayni 1998] B. Ghusayni, "Some representations of $\zeta(3)$", *Missouri J. Math. Sci.* **10**:3 (1998), 169–175.

[Lewin 1981] L. Lewin, *Polylogarithms and associated functions*, North-Holland, New York, 1981.

[Lewin 1991] L. Lewin (editor), *Structural properties of polylogarithms*, edited by L. Lewin, Math. Surv. Monographs **37**, Amer. Math. Soc., Providence, RI, 1991.

[Remiddi and Vermaseren 2000] E. Remiddi and J. A. M. Vermaseren, "Harmonic polylogarithms", *Internat. J. Modern Phys. A* **15**:5 (2000), 725–754. Preprint available at www.arxiv.org/abs/hep-ph/9905237.

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