Central Binomial Sums, Multiple Clausen Values and Zeta Values

Jonathan Michael Borwein, FRSC
Shrum Chair of Science
Department of Mathematics and Statistics
Simon Fraser University, Burnaby, BC V5A 1S6 Canada
e-mail: jborwein@cecm.sfu.ca

David J. Broadhurst
Physics Department
Open University, Milton Keynes, MK7 6AA, UK
e-mail: D.Broadhurst@open.ac.uk

Joel Kamnitzer
Department of Applied Mathematics
University of Waterloo, Waterloo, ON N2L 3G6 Canada
e-mail: jkamnitz@uwaterloo.ca

3 April 2000

Abstract
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 non-alternating 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. In the non-alternating case, there is a strong connection to polylogarithms of the sixth root of unity, encountered in the 3-loop Feynman diagrams of hep-th/9803091 and subsequently in hep-ph/9910223, hep-ph/9910224, cond-mat/9911452 and hep-th/0004010.

Key words: binomial sums, multiple zeta values, log-sine integrals, Clausens function, multiple Clausen values, polylogarithms, Apéry sums.
1 Introduction

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

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

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 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 [10].

We shall finish by discussing the corresponding alternating sum:

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

These are related to polylogarithmic ladders in the golden ratio $\frac{\sqrt{5} - 1}{2}$. A classical evaluation is $A(3) = \frac{2}{5} \zeta(3)$, with its connections to Apéry's proof of the irrationality of $\zeta(3)$, (see e.g., [5]).

2 Definitions and Preliminaries

We start with some definitions which for the most part follow Lewin [14], and [6, 7, 8]. A useful multi-dimensional polylogarithm is defined by

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

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

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

$$\mu(a_1, \ldots, a_k) := Li_{a_1, \ldots, a_k}(\omega).$$

This MCV is analogous to the multiple zeta value (MZV), at $z = 1$, which has been studied in works such as [6, 7, 8]. We might also have viewed these 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:

$$\text{mgl}(a_1, \ldots, a_k) := \text{Re}(i^{n_1 + \cdots + n_k} \mu(a_1, \ldots, a_k))$$
$$\text{mcl}(a_1, \ldots, a_k) := \text{Im}(i^{n_1 + \cdots + n_k} \mu(a_1, \ldots, a_k)).$$
and may be written explicitly as multiple \sin or \cos sums depending on the parity. For example, when \(a + b\) is odd,

\[
\text{mg}l(a, b) = \pm \sum_{n,m > 0} \frac{\sin(n \frac{\pi}{2})}{n^a m^b},
\]
as is the case in Theorem 1 below.

As elsewhere, the \textit{weight} of a sum is \(\sum_{i=1}^{k} a_i\) while the \textit{depth} \(k\) is the number of parameters. This separation corresponds, in the case \(k = 1\), to Lewin’s ([14]) separation of the polylogarithm at complex exponential arguments into Clausen and Glaisher functions.

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

\[
\frac{d \text{Li}_{a_1+2,a_2,\ldots,a_n}(z)}{dz} = \frac{\text{Li}_{a_1+1,\ldots,a_n}(z)}{z},
\]

\[
(3)
\]
\[
\frac{d \text{Li}_{a_1,a_2,\ldots,a_n}(z)}{dz} = \frac{\text{Li}_{a_2,\ldots,a_n}(z)}{1-z},
\]

\[
(4)
\]
Repeated application of (4) yields:

\[
\text{Li}_{\{1\}^n}(z) = \left(\frac{-\log(1-z)}{n!}\right)^n,
\]

\[
(5)
\]

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

We will make some use of the \textit{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 \textit{nth Bernoulli number} and is written \(B_n\).

For convenience we choose the following notation for \textit{log-sine integrals}. We define

\[
j(a, b) := \int_0^{\pi/3} (\log(2 \sin \frac{\theta}{2}))^a \theta^b d\theta
\]

\[
(6)
\]

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

\[
(7)
\]

Finally, note the following standard result involving the \textit{Gamma function} which will prove very useful:

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

3
3 Non-alternating Central Binomial Sums

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

**Lemma 1** For all positive integers

$$S(k) = \frac{(-2)^{k-2}}{(k-2)!} j(k-2, 1). \quad (8)$$

**Proof.** Employing the Gamma function and various standard tricks, we have:

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

$$= \sum_{n=1}^{\infty} \frac{1}{2n(n \pi)^k} \int_{0}^{1} (-\log x)^{k-1} x^{n-1} dx$$

$$= \sum_{n=1}^{\infty} \frac{1}{2n(n \pi)^k} \int_{0}^{1} (-2 \log y)^{k-1} y^{2n-2} (2y) dy \quad \text{(by } y^2 = x)$$

$$= -\sum_{n=1}^{\infty} \frac{(-2)^{k-1}}{2n(n \pi)^k} \left( \int_{0}^{1} \frac{y^{2n}}{2n} \frac{(\log y)^{k-2}}{y} dy \right)$$

(after integrating by parts)

$$= \frac{(-2)^{k-1}}{(k-2)!} \int_{0}^{1} \frac{(\log y)^{k-2}}{y} \sum_{n=1}^{\infty} \frac{y^{2n}}{n2n(n \pi)^k} dy$$

$$= \frac{(-2)^{k-1}}{(k-2)!} \int_{0}^{1} \frac{(\log y)^{k-2}}{y} \frac{y \arcsin \frac{\theta}{2}}{\sqrt{1 - (\frac{\theta}{2})^2}} d\theta \quad \text{(see [5] p. 384)}$$

$$= \frac{(-2)^{k-2}}{(k-2)!} \int_{0}^{\pi/3} (\log(2 \sin \theta)^{k-2} d\theta \quad \text{(by } y = 2 \sin \frac{\theta}{2}).$$

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 2** For all $k > 2$,

$$\sum_{r=0}^{k-2} \frac{(-i \pi/3)^r}{r!} \mu(k-r, \{1\}^n) = \zeta(k, \{1\}^n) - (-1)^{k+n} r(n+1, k-2). \quad (9)$$

**Proof.** First note the formal identity:

$$\log(1 - e^{i \theta}) = \log \left( 2 \sin \frac{\theta}{2} \right) + \frac{i}{2} (\theta - \pi). \quad (10)$$

We have

$$\mu(k, \{1\}^n) = \zeta(k, \{1\}^n) + \int_{1}^{\infty} \frac{\text{Li}_{k-1, \{1\}^n}(z)}{z} dz \quad \text{(by } (3)).$$
We now integrate by parts repeatedly to obtain:

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

Observe that $\log(\omega) = \frac{i\pi}{3}$. Let $z = e^{i\theta}$. Then we have (using (5)):

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

which gives us the desired result after applying (10).

Now, note that $r(a, b)$, defined in (7), can be expanded out binomially and written as linear rational combination of $j(c, d)$, defined in (6), for various $c, d$, including a non-zero 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 $\text{mcl}(n, \{1\}^r), \text{mgl}(n, \{1\}^r)$ and $\zeta(n, \{1\}^r)$.

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 both Reduce and 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 results:

**Theorem 1** The following evaluations of central binomial sums hold:

\begin{align*}
S(2) &= \frac{\zeta(2)}{3} \\
S(3) &= -\frac{2\pi}{3} \text{mcl}(2) - \frac{4}{3} \zeta(3) \\
S(4) &= \frac{17}{36} \zeta(4) \\
S(5) &= 2\pi \text{mcl}(4) - \frac{19}{3} \zeta(5) + \frac{2}{3} \zeta(3) \zeta(2) \\
S(6) &= -\frac{4\pi}{3} \text{mgl}(4, 1) + \frac{3341}{1296} \zeta(6) - \frac{4}{3} \zeta(3)^2 \\
S(7) &= -6\pi \text{mcl}(6) - \frac{493}{24} \zeta(7) + 2\zeta(5) \zeta(2) + \frac{17}{18} \zeta(4) \zeta(3) \\
S(8) &= -4\pi \text{mgl}(6, 1) + \frac{3462601}{233280} \zeta(8) - \frac{14}{15} \zeta(5, 3) - \frac{38}{3} \zeta(5) \zeta(3) + \frac{2}{3} \zeta(2) \zeta(3)^2.
\end{align*}
Note that the results for $S(2)$ and $S(4)$ are classical evaluations. The others are new and it is hoped that they will shed light on odd $\zeta$-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 $n \leq 20$ through a very high level application of integer relation algorithms. The result for $S(20)$ is presented in [2].

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 the following results about depth-one Clausen values as described in [14]:

\[ \text{mgl}(n) = \frac{(-1)^{n+1}2^{2n-1}B_n(\frac{1}{2})}{n!}, \quad (11) \]
\[ \text{mcl}(2n + 1) = \frac{(-1)^n}{2}(1 - 2^{-2n})(1 - 3^{-2n})\zeta(2n + 1). \quad (12) \]

4.1 MCV Duality

In MZV analysis, one of the central results is the now well-known MZV duality theorem recapitulated in [6]:

\[ \zeta(a_1 + 2, \{1\}_b_1, \ldots, a_k + 2, \{1\}_b_k) = \zeta(b_k + 2, \{1\}_a_k, \ldots b_1 + 2, \{1\}_a_1), \quad (13) \]

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

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 2 is somewhat complicated. A prior example may make things clearer.

Example 1

\[
\mu(1, 3, 1, 2) - \mu(1)\mu(1, 1, 2) + \mu(2)\mu(2, 1, 2) - \mu(3)\mu(1, 1, 2) + \mu(1, 3)\mu(1, 2) - \mu(1, 1, 3)\mu(2) + \mu(2, 1, 3)\mu(1) - \mu(1, 2, 1, 3) = 0.
\]

Note that each term differs from the previous 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 2  For all positive integers \(a_1, a_2, \ldots, a_n\)

\[
\mu(1, a_1, \ldots, a_n) - \mu(1)^2 \mu(a_1, \ldots, a_n) + \mu(2)^2 \mu(a_1 - 1, \ldots, a_n) + \ldots \\
\pm \mu(1)a_1 \mu(a_2, \ldots, a_n) + \mu(1, a_2, \ldots, a_n) + \ldots \pm \mu(1, a_n, \ldots, a_1) = 0.
\]

(14)

Proof. We will prove this by repeated integration by parts. We use the differential properties (3) and (4) to move weight from one multidimensional polylogarithm to another:

\[
\mu(1, a_1, \ldots, a_n) = \int_0^\infty \frac{L_{a_1, \ldots, a_n}(z)}{1 - z} dz \\
= [L_{11}(z) L_{a_1, \ldots, a_n}(z)]_0^\infty - \int_0^\infty \frac{L_{11}(z) L_{a_1 - 1, \ldots, a_n}(z)}{z} dz \\
\ldots \\
= \ldots \pm \mu(1, a_n, \ldots, a_1).
\]

As in other duality results, it is interesting to examine what happens in the self-dual case. Suppose that \((a_1, \ldots, a_n) = (a_n, \ldots, a_1)\), then if \(a_1 + \cdots + a_n\) is even, (14) reduces to 0 = 0. If the sum is odd, then (14) shows that \(\mu(1, a_1, \ldots, a_n)\) reduces to a sum and product of lower weight MCVs.

The pattern in Theorem 3 below is somewhat more complicated. Hence an example will be even more instructive. (The bar denotes complex conjugation.)

Example 2

\[
\mu(4, 3, 1) + \overline{\mu(1)^2 \mu(3, 3, 1) + \mu(1, 1)^2 \mu(2, 3, 1) + \mu(1, 1)^2 \mu(3, 1)} \\
+ \mu(2, 1, 1) \mu(3, 1) + \mu(1, 2, 1, 1) \mu(2, 1) + \mu(1, 1, 2, 1, 1) \mu(1, 1) \\
+ \mu(2, 1, 2, 1, 1) \mu(1) + \overline{\mu(3, 1, 2, 1, 1)} = \zeta(3, 1, 2, 1, 1).
\]

Note that each term differs from the previous 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 3  For all positive integers \(a_1, a_2, \ldots, a_n\)

\[
\mu(a_1 + 2, \{1\}_b, \ldots, a_k + 2, \{1\}_b) + \mu(1)^2 \mu(a_1 + 1, \{1\}_b, \ldots, a_k + 2, \{1\}_b) + \ldots \\
\overline{\mu(a_1 + 1, \{1\}_b, \ldots, a_k + 2, \{1\}_b) + \mu(2, 1, \{1\}_a) \mu(\{1\}_b, \ldots, a_k + 2, \{1\}_b)} \\
\overline{\ldots + \mu(1) \mu(a_2, \ldots, a_k + 2, \{1\}_b) + \mu(1, 1) \mu(a_2, \ldots, a_k + 2, \{1\}_b) + \ldots \\
\overline{\mu(b_k + 2, \{1\}_a, \ldots b_1 + 2, \{1\}_a) = \zeta(b_k + 2, \{1\}_a, \ldots b_1 + 2, \{1\}_a)}}
\]

(15)
Proof. As stated above, this follows by Hölder convolution, since \( \text{Li}_d(x) = \mu(a) \).

It can also be proved using a similar integration by parts as above, after noting that the following differentiation result holds:

\[
\frac{d \text{Li}_{a_1+a_2+\ldots+a_n}(1-z)}{dz} = -\frac{\text{Li}_{a_1+1,a_2,\ldots,a_n}(1-z)}{1-z}
\]

\[
\frac{d \text{Li}_{a_2,\ldots,a_n}(1-z)}{dz} = -\frac{\text{Li}_{a_2,\ldots,a_n}(1-z)}{z}
\]

This identity allows us to move weight from a multi-dimensional polylogarithm at \( z \) to one at \( 1-z \).

Note that 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 (15) will vanish, since \( a\pi + \pi b \) is real. When \( k = 1 \), (15) simplifies to the following, on using (11),

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

We initially derived (16) by means of (9) and the following satisfying identity involving log-sine integrals, which we proved using contour integration:

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

4.2 Special values of MCVs

To illustrate the utility of this last duality result, consider (16) when \( a = 1 \) and \( b = 1 \). We obtain:

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

Using MZV analysis [8], we know that \( \zeta(3,1) = \frac{2\pi^2}{324} \), which is the first case in an infinite series of evaluations in terms of powers of \( \pi^2 \), conjectured by Zagier and proved in [7]. Now from (21) below we have

\[
\text{mgl}(2,1) = \frac{\pi^3}{324}.
\]

This rewards us with

\[
\text{mgl}(3,1) = \frac{-23}{19440} \pi^4.
\]
Next, let us use the duality result to extract some more general evaluations. Let
\[
F(x, y) := \sum_{a, b \geq 0} \mu(a + 2, \{1\}_b) x^{a+1} y^{b+1}.
\]
According to [8], we know that this generating function is hypergeometric:
\[
F(x, y) = 1 - 2 F_1(-x, y; 1 - x; \omega).
\] (18)

Unfortunately, this is not a very convenient equation for extracting coefficients or proving formulas. To obtain a more useful representation, we take (16), multiply through by \(x^{a+1} y^{b+1}\) and sum over all \(a, b \geq 0\). This gives:
\[
e^{-i\pi x/3} F(x, y) + e^{i\pi y/3} F(y, x) + (e^{-i\pi x/3} - 1)(e^{i\pi y/3} - 1) = G(x, y),
\] (19)
where
\[
G(x, y) := \sum_{a, b \geq 0} \zeta(a + 2, \{1\}_b) x^{a+1} y^{b+1}
\]
is the generating function for the corresponding MZVs. Now from prior work on MZVs (see [6]) it is known that
\[
G(x, y) = 1 - \exp \left( \sum_{k \geq 2} \frac{x^k + y^k - (x+y)^k}{k} \zeta(k) \right).
\]
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 \(M(x, y) :=\)
\[
F(ix, -iy) = \sum_{a, b \geq 0} (-1)^{b+1} (\text{mgl}(a + 2, \{1\}_b) + i \text{mcl}(a + 2, \{1\}_b)) x^{a+1} y^{b+1}.
\]
Then we have:
\[
e^{\pi x/3} M(x, y) + e^{\pi y/3} M(y, x) + (e^{\pi x/3} - 1)(e^{\pi y/3} - 1) = G(ix, -iy).
\] (20)

**Theorem 4** For non-negative integers \(a\) and \(b\)
\[
\text{mgl}(\{1\}_a, 2, \{1\}_b) = (-1)^{a+b+1} \frac{(\frac{a+b+2}{3})^{a+b+2}}{2(a+b+2)!}.
\] (21)

and depends only on \(a + b\).

**Proof.** First we show that
\[
\text{mgl}(2, \{1\}_b) = (-1)^{b+1} \frac{(\frac{3}{2})^{b+2}}{2(b+2)!}.
\]
We give two proofs of this result.
(i) Multiply by \( \frac{y}{x} \) in (20), and let \( x \) go to zero. Set \( B(y) := \sum_{b=0}^{\infty} (-1)^{b+1} \mathrm{mgl}(2, \{1\}_b)y^{b+2} \),

\[ C(y) := \sum_{b=0}^{\infty} (-1)^{b+1} \mathrm{mgl}(b+2)y^{b+2} \]

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

Comparing real parts on each side of (20) yields

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

The value of \( \mathrm{mgl}(n) \) and so of \( C(y) \) is given by (11), 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:

\[ B(y) = \frac{e^{\pi y/3}}{2} - \frac{\pi y}{6} - \frac{1}{2} \Rightarrow \mathrm{mgl}(2, \{1\}_b) = (-1)^{b+1} \frac{(\frac{\pi y}{3})^{b+2}}{2(b+2)!}. \]

(ii) Alternatively, we start with (18). Dividing by \( x \), setting \( y = iy \), and letting \( x \) go to zero yields:

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

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 \( \omega \) along \( z = 1 + e^{i(\pi - \theta)} \), \( \frac{2\pi}{4} \leq \theta \leq \pi \), to obtain,

\[ \sum_{n=1}^{\infty} \frac{(iy)_n \omega^n}{n n!} = -i \left( \int_0^{\frac{\pi}{4}} \frac{(e^{-\theta y} - 1)(1 - \cos \theta + i \sin \theta)}{2 - 2\cos \theta} d\theta + \frac{e^{-\pi y/3}y}{y} - 1 \right). \]

This again gives us:

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

as required.

Armed with this special case, we now prove the full result for \( \mathrm{mgl}(\{1\}_a, 2, \{1\}_b) \).
We start with a similar integration by parts as for the proof of (9). We have:

\[
\mu(\{1\}_{b}, 2, \{1\}_{a}) = \int_{0}^{\infty} \frac{Li(1)_{b-1, 2, (1)_{a}}(z)}{1 - z} \, dz \\
= \frac{i\pi}{3} \mu(\{1\}_{b-1}, 2, \{1\}_{a}) + \cdots + (-1)^{b+1} \frac{(i\pi)^{b}}{b!} \mu(2, \{1\}_{a}) \\
+ \int_{0}^{\infty} \frac{(\log(1 - z))^{b} Li_{1}(z)}{b!z} \, dz
\]

(by repeated integration by parts)

\[
= \frac{i\pi}{3} \mu(\{1\}_{b-1}, 2, \{1\}_{a}) + \cdots + (-1)^{b+1} \frac{(i\pi)^{b}}{b!} \mu(2, \{1\}_{a}) \\
+ (-1)^{b} a + b + 1 \mu(2, \{1\}_{a+b}) \quad \text{using (5).}
\]

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

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

However, \(a + b + 2(0) = a + b + 1(0) + a + b + 1(0) = 1\) and it is now easily seen that the left-side telescopes.

### 4.3 Additional Evaluations

We can use (20) to obtain a clean expression for the alternating sum of all mgf’s of the form mgf(\(a, \{1\}_{b}\)) of fixed weight. Let

\[
A(x) := \sum_{n=1}^{\infty} \left( \sum_{m=0}^{n-2} (-1)^{m+1} \text{mgf}(n + 2 - m, \{1\}_{m}) \right) x^{n}.
\]

If we set \(x = y\) in (20) then, after some work, we obtain

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

This leads to

\[
\sum_{m=0}^{n-2} (-1)^{m+1} \text{mgf}(n + 2 - m, \{1\}_{m}) = \frac{-\pi^{n}}{2n!} \left( B_{n} \left( \frac{1}{3} \right) 2^{n} + \left( \frac{1}{3} \right)^{n} \right). \quad (22)
\]

We note that (22) is equivalent to

\[
\text{Re} \left( 1_{2}F_{1}(-ix, -ix; 1; -ix; \omega) \right) = \text{Re} \left( \sum_{n=1}^{\infty} \frac{(-ix)^{n}}{n - ix} \omega^{n} \right) = -\frac{1}{2} \left( \frac{\pi xe^{-\pi x/3}}{\sinh(\pi x) + e^{\pi x}} - 2 \right).
\]
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 (18) 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 $\zeta$-evaluations [9]). For example, extracting the coefficient of $x$ yields:

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

More generally, we obtain

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

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 [11], 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 $\pi$ are those already identified, namely $\text{mgl}(3, 1)$ and $\text{mgl}((1)_b, 2, \{1\}_a)$. Moreover we found no other non-trivial 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 $C(n) := \{\text{mcl}(a_1, \ldots, a_k) : a_1 + \cdots + a_k = n\}$ of all multiple Clausen values of fixed weight, $n$. We wish to determine the smallest set of real numbers such that each element of $C(n)$ 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 $\pi$. We denote by $I(n)$ the size of the basis for $C(n)$. Similarly, we denote by $R(n)$ the basis size for multiple Glaisher values of weight $n$.

Our first conjecture is quite striking:

**Conjecture 1** The following twisted Fibonacci recursion obtains:

$$R(n) = R(n - 1) + I(n - 2)$$
$$I(n) = I(n - 1) + R(n - 2)$$
$$R(0) = R(1) = 1 \text{ and } I(0) = I(1) = 0.$$
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 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 [2] for $k \leq n \leq 7$. They provide compelling evidence that there is a great deal of structure to MCVs. It seems unlikely that they will be proven 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 used, at

http://www.cecm.sfu.ca/projects/EZFace/Java/

and in a forthcoming CECM interface for more general integer relation problems.

### 6 Apéry Sums and the Golden Ladder

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

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

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 [15].

The results for $k < 5$ were proven by classical methods (and also obtained by John Zucker, private communication). For $k \geq 5$, we were content to rely on the empirical methods adopted in [15], determining rational coefficients from high precision numerical computations.
At \( k = 2 \) one easily obtains from Clausen’s hypergeometric square, given in
[1] or [5], the result
\[
A(2) = 2L^2
\]
where
\[
L := \log(\rho).
\]
Indeed, we found 6 integer relations between \( A(2), \zeta(2) \), and the dilogarithms
\( \{\text{Li}_2(\rho^p) \mid p \in \mathbb{C} \} \), where
\[
\mathbb{C} := \{ 1, 2, 3, 4, 6, 8, 10, 12, 20, 24 \}
generates the corresponding cyclotomic relations [15].

In general, it is more convenient to work with the set
\[
K_k := \{ L_k(\rho^p) \mid p \in \mathbb{C} \}
\]
of Kummer-type polylogarithms, of the form
\[
L_k(x) := \frac{1}{(k-1)!} \int_0^x \frac{(-\log |y|)^{k-1}dy}{1-y} = \sum_{r=0}^{k-1} \frac{(-\log |x|)^r}{r!} \text{Li}_{k-r}(x)
\]
where as before \( \text{Li}_k(x) := \sum_{n>0} x^n/n^k \).

At \( k = 3 \) one has Apéry’s result
\[
A(3) = \frac{2}{3}\zeta(3).
\]
Moreover there are 5 integer relations between \( K_3, L^3, \) and \( \zeta(3) \).

At \( k = 4 \) we recently proved a result, using classical polylogarithmic theory, which simplifies to
\[
A(4) = 4\overline{L}_4(\rho) - \frac{1}{2}L^4 - 7\zeta(4)
\]
where
\[
\overline{L}_k(x) := L_k(x) - L_k(-x) = 2L_k(x) - 2^{1-k}L_k(x^2).
\]
In fact, there are 5 integer relations between \( K_4, L^4, \zeta(4) \) and \( A(4) \). Another simple example is
\[
A(4) = \frac{11}{8}\overline{L}_4(\rho^2) - 2L^4 - \frac{23}{4}\zeta(4).
\]

At \( k = 5 \) we found 4 empirical integer relations between \( K_5, L^5, \zeta(5) \) and \( A(5) \). The simplest result is
\[
A(5) = \frac{7}{2}L_5(\rho^2) + \frac{1}{5}L^5 - 2\zeta(5).
\]
More explicitly, with \( \rho := (\sqrt{5} - 1)/2 \), this produces
\[
\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5\binom{2k}{k}} = 2\zeta(5) - \frac{4}{5}\log(\rho)^5 + \frac{8}{5}\log(\rho)^3\zeta(2) + 4\log(\rho)^2\zeta(3)
\]
\[
+ 80 \sum_{n>0} \left( \frac{1}{(2n)^5} - \frac{\log(\rho)}{(2n)^2} \right) \rho^{2n},
\]
(23)
which, along with previous integer relation exclusion bounds (see, e.g., [4], [10]), helps explain why no ‘simple’ evaluation for \( A(5) \) such as those for \( S(2), A(3), S(4) \) has ever been found.

At \( k = 6 \) we found the empirical relation

\[
11 \{ A(6) - \frac{2}{3} \zeta^2(3) \} = 144 \bar{L}_6(\rho) - \frac{64}{9} \bar{L}_6(\rho^3) + \frac{2}{9} L^6 - \frac{244}{9} \zeta(6)
\]

which is the simplest of 3 integer relations between \( K_6, L^6, \zeta(6) \) and the combination \( A(6) - \frac{2}{3} \zeta^2(3) \).

At \( k = 7 \) there are 2 integer relations between \( K_7, L^7 \), 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

\[
2791022262 \zeta(9) = 15750 L_9(\rho^{24}) + 74277 L_9(\rho^{20}) - 8750000 L_9(\rho^{12}) - 19014912 L_9(\rho^{10}) - 206671500 L_9(\rho^8) + 1295616000 L_9(\rho^6) - 3180657175 L_9(\rho^4) + 4907952000 L_9(\rho^2) - 525376000 \log^3(\rho).
\]

This still falls short of the ladder for \( \zeta(11) \), in [12]. The current record is set by the ladder for \( \zeta(17) \) in [3], which extends the weight-16 analysis of Henri Cohen, Leonard Lewin and Don Zagier [13], in the number field of the Lehmer polynomial of conjecturally smallest Mahler measure.

**Acknowledgements.** This research was in part performed while Joel Kamnitzer was an NSERC Undergraduate Research Fellow at CECM in 1999 and while David Broadhurst visited CECM. For this and other direct NSERC support to Dr Borwein we express our gratitude.

We also wish to thank Simon Plouffe and Philippe Flajolet for communications which triggered some of our explorations, and David Bailey, David Bradley, Petr Lisonek and John Zucker for many useful exchanges.
References


