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Mahler measures, short walks and log-sine integrals

Jonathan M. Borwein* and Armin Straub†

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Abstract

The Mahler measure of a polynomial in several variables has been a subject of much study over the past thirty years — very few closed forms are proven but more are conjectured. In the case of multiple Mahler measures more tractable but interesting families exist. Using values of log-sine integrals we provide systematic evaluations of various higher and multiple Mahler measures.

The evaluations in terms of log-sine integrals become particularly useful in light of the fact that log-sine integrals may be automatically reexpressed as polylogarithmic values. We present this correspondence along with related generating functions for log-sine integrals.

Our initial interest in considering Mahler measures stems from a study of uniform random walks in the plane as first introduced by Pearson. The main results on the moments of the distance traveled by an n -step walk, as well as the corresponding probability density functions, are reviewed. It is the derivative values of the moments that are Mahler measures.

This work would be impossible without very extensive symbolic and numeric computations. It also makes frequent use of the new NIST Handbook of Mathematical Functions and similar tools. Our intention is to show off the interplay between numeric and symbolic computing while exploring the three mathematical topics in the title.

*Centre for Computer-assisted Research Mathematics and its Applications (CARMA), School of Mathematical and Physical Sciences, University of Newcastle, Callaghan, NSW 2308, Australia, jonathan.borwein@newcastle.edu.au. Distinguished Professor King Abdulaziz University, Jeddah.

†Tulane University, New Orleans, LA 70118, USA. Email: astraub@tulane.edu

1 Introduction

The *multiple Mahler measure* [31] of k functions P_1, \dots, P_k (typically Laurent polynomials) in n variables is defined as

$$\mu(P_1, P_2, \dots, P_k) = \int_0^1 \cdots \int_0^1 \prod_{j=1}^k \log |P_j(e^{2\pi i t_1}, \dots, e^{2\pi i t_n})| dt_1 dt_2 \cdots dt_n. \quad (1)$$

When $k = 1$ this reduces to the standard (logarithmic) *Mahler measure* [16] which, while introduced by Mahler in 1923, has been a subject of much study over the past thirty years. One of its basic properties is that the map $M_1 : P \mapsto \exp \mu(P)$ is multiplicative. If $n = 1$ then $M_1(P) = 1$ if and only if P is a product of cyclotomic polynomials. For other polynomials, Lehmer's conjecture (1931) asserts that the smallest Mahler measure is attained by $1 - x + x^3 - x^4 + x^5 - x^6 + x^7 - x^9 + x^{10}$.

$\mu(P)$ turns out to be an example of a *period*. When $n = 1$ and P has integer coefficients then $M_1(P)$ is an algebraic integer. In several dimensions life is harder. We shall see remarkable recent results such as (58) — many more discovered than proven — expressing $\mu(P)$ arithmetically.

In the case that $P = P_1 = P_2 = \cdots = P_k$, the definition (1) devolves to the *higher Mahler measure* $\mu_k(P)$ as introduced and examined in [31]. A natural source for a family of higher Mahler measures was met by the authors in their recent study of random walks in the plane: an n -step uniform random walk starts at the origin and consists of n steps of length 1 each taken into a uniformly random direction. The study of such walks largely originated with Pearson more than a century ago [38, 37, 39] who posed the problem of determining the distribution of the distance from the origin after a certain number of steps. The s -th moment of the distance traveled by an n -step uniform random walk is given by

$$W_n(s) = \int_0^1 \cdots \int_0^1 \left| \sum_{k=1}^n e^{2\pi i t_k} \right|^s dt_1 \cdots dt_n. \quad (2)$$

These moments have been studied in [11, 14], while the (radial) densities p_n of the distance traveled in n steps have been the subject of [15]. The main results will be presented in Section 2.

The expected value $W_1(1)$ is trivially 1, and one easily finds $W_2(1) = \frac{4}{\pi}$. For $n \geq 3$, however, the evaluation of $W_n(1)$ becomes rather nontrivial — while for $n \geq 5$ it is not well understood at all. The same may be said for the determination of the densities p_n . More generally, similar problems — e.g., Bessel moments, Box integrals, Ising integrals — tend to get much more difficult in five or more dimensions.

Even from a purely numerical point of view, the integrals (2) are challenging without further insight or treatment. In fact, $W_5 \approx 2.0081618$ was the best estimate we could compute *directly* on 256 cores at Lawrence Berkeley National Laboratory. Bailey and the first author have a general project to develop symbolic numeric techniques for (meaningful) multi-dimensional integrals.

The moments $W_n(s)$, generalized to the situation of walks with varying but prescribed step lengths, are also studied in [42] and various presentations are given for them. The reason for their appearance in [42] is a relation with Mahler measures: in light of (1), one observes that (multiple) derivatives of W_n evaluated at zero are (multiple) Mahler measures. In particular,

$$W'_n(0) = \mu(x_1 + x_2 + \dots + x_n) = \mu(1 + x_1 + \dots + x_{n-1}) \quad (3)$$

and, more generally,

$$W_n^{(k)}(0) = \mu_k(1 + x_1 + \dots + x_{n-1}). \quad (4)$$

A multiple Mahler measure, similar to the case $n = 3$, was studied by Sasaki [44, Lemma 1], who considered

$$\mu_k(1 + x + y_*) := \mu(1 + x + y_1, 1 + x + y_2, \dots, 1 + x + y_k) \quad (5)$$

and provided an evaluation of $\mu_2(1 + x + y_*)$. As observed in [12] this Mahler measure can be conveniently expressed in terms of *log-sine integrals*. Namely, if

$$\text{Ls}_n^{(k)}(\sigma) = - \int_0^\sigma \theta^k \log^{n-1-k} \left| 2 \sin \frac{\theta}{2} \right| d\theta \quad (6)$$

denotes the (generalized) log-sine integral [33], then

$$\mu_k(1 + x + y_*) = \frac{1}{\pi} \text{Ls}_{k+1} \left(\frac{\pi}{3} \right) - \frac{1}{\pi} \text{Ls}_{k+1}(\pi). \quad (7)$$

Many other Mahler measures studied in [12, 4] were shown to have evaluations involving generalized log-sine integrals at π and $\pi/3$ as well. Several such examples are reviewed in Section 3. The advantage of expressing Mahler measures in terms of log-sine integrals is that the latter may be evaluated systematically and automatically as polylogarithmic values. This is described in Section 4, which discusses log-sine integrals and their evaluations, both explicit and in terms of generating series. Many examples of evaluations of log-sine integrals and their history are collected in [19],

which then establishes several families of evaluations for log-sine integrals with a focus on the argument $\pi/3$. Subsection 4.1 concludes with an indication of the physical importance of log-sine integrals.

We wish to emphasize that, almost without exception, every new result was found through a mixture of symbolic and numeric computing along with a great deal of graphic computing: call this *SNaG*. In particular, we note that many of the innocent looking real line plots are the result of a subtle interplay of symbolic and numeric calculation. Many results were discovered from and in the course of the creation of these pictures. Moreover, neither author really trusts a result until it has been checked numerically to high precision and if possible symbolically.

We close this introduction by presenting some of the notations used for special functions throughout this manuscript. The *multiple polylogarithm* as studied for instance in [8] and [5, Ch. 3] will be denoted by

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

The *depth* of this polylogarithm refers to k while its *weight* is $w = a_1 + \dots + a_k$. For our purposes, the a_1, \dots, a_k will usually be positive integers and $a_1 \geq 2$ so that the sum converges for all $|z| \leq 1$. For example,

$$\text{Li}_{2,1}(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2} \sum_{j=1}^{k-1} \frac{1}{j}.$$

In particular, $\text{Li}_k(x) := \sum_{n=1}^{\infty} \frac{x^n}{n^k}$ is the *polylogarithm of order k* . The usual notation will be used for repetitions so that, for instance, $\text{Li}_{2, \{1\}^3}(z) = \text{Li}_{2,1,1,1}(z)$.

An important special case are the *multiple zeta values* which will be denoted by

$$\zeta(a_1, \dots, a_k) := \text{Li}_{a_1, \dots, a_k}(1).$$

More generally, we will be interested in polylogarithms at roots of unity. In accordance with [33], these are split into *multiple Clausen functions* (Cl) and *multiple Glaisher functions* (Gl), defined as

$$\text{Cl}_{a_1, \dots, a_k}(\theta) = \left\{ \begin{array}{ll} \text{Im Li}_{a_1, \dots, a_k}(e^{i\theta}) & \text{if } w \text{ even} \\ \text{Re Li}_{a_1, \dots, a_k}(e^{i\theta}) & \text{if } w \text{ odd} \end{array} \right\}, \quad (8)$$

$$\text{Gl}_{a_1, \dots, a_k}(\theta) = \left\{ \begin{array}{ll} \text{Re Li}_{a_1, \dots, a_k}(e^{i\theta}) & \text{if } w \text{ even} \\ \text{Im Li}_{a_1, \dots, a_k}(e^{i\theta}) & \text{if } w \text{ odd} \end{array} \right\}. \quad (9)$$

Our other notation and usage is largely consistent with that in [33] and that in the newly published [36], in which most of the requisite material is described. Finally, a recent elaboration of what is meant when we speak about evaluations and “closed forms” is to be found in [10].

2 Short random walks

2.1 General moments of random walks

The term “random walk” first appears 1905 in a question by Karl Pearson in *Nature* [38] where he considers the following problem:

“A man starts from a point O and walks l yards in a straight line; he then turns through any angle whatever and walks another l yards in a second straight line. He repeats this process n times. I require the probability that after these n stretches he is at a distance between r and $r + \delta r$ from his starting point, O .”

This triggered a response by Lord Rayleigh [40] just one week later. Rayleigh replied that he had considered the problem earlier in the context of the composition of vibrations of random phases, and gave the approximate probability density $\frac{2x}{n}e^{-x^2/n}$ for the distance traveled in n steps of unit length if n is large.

Another week later, Pearson again wrote in *Nature*, see [37], to note that G. J. Bennett had given a solution for the probability distribution for $n = 3$, which can be written in terms of the analytic continuation of K , the *complete elliptic integral* of the first kind. Namely, the density function $p_3(x)$, for $0 \leq x \leq 3$, can be written as

$$p_3(x) = \operatorname{Re} \left(\frac{\sqrt{x}}{\pi^2} K \left(\sqrt{\frac{(x+1)^3(3-x)}{16x}} \right) \right), \quad (10)$$

see, e.g., [29] and [39]. This expression, while analytically correct, is very hard to use both numerically and symbolically, and somewhat mysterious. We shall provide two more satisfactory expressions in equations (37) and (38) of Section 2.4.

Pearson also concluded that there was still great interest in the case of small n which, as he had noted, is dramatically different from that of large n . This is illustrated in Figure 1: while p_8 is visually almost indistinguishable from the smooth limiting density $\frac{2x}{n}e^{-x^2/n}$ (shown in superimposed dotted lines) given by Rayleigh, the densities p_3 , p_4 and p_5 have remarkable features of their own.

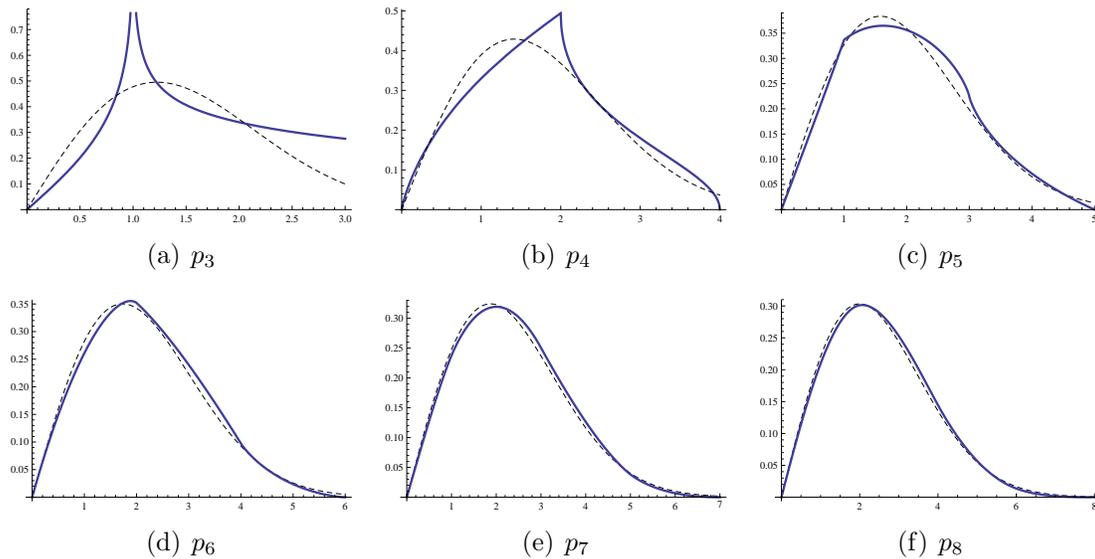


Figure 1: Densities p_n with the limiting behaviour superimposed

Before returning to the densities p_n we will discuss the moments $W_n(s)$ of the distance traveled in n steps. While their interpretation gives rise to the multiple integral representation (2), they may be expressed in terms of the density functions as

$$W_n(s) = \int_0^\infty x^s p_n(x) dx. \quad (11)$$

In other words, $W_n(s-1)$ is the *Mellin transform* of p_n , see e.g. [35]. We denote this by $W_n(s-1) = \mathcal{M}[p_n; s]$. Conversely, the density p_n is the *inverse Mellin transform* of $W_n(s-1)$. In particular, the moment function $W_n(s)$ determines the density $p_n(x)$.

In fact, much more is true. To this end, we wish to remind the reader of Carlson's Theorem [49, 5.81], which enables the transition from the discrete to the continuous and which lies under much of what follows. A function f is said to be of *exponential type* in a region if, in that region, $|f(z)| \leq M e^{c|z|}$ for some constants M and c .

Theorem 2.1 (Carlson). *Let f be analytic in the right half-plane $\operatorname{Re} z \geq 0$ and of exponential type. Assume further that, on the imaginary axis $\operatorname{Re} z = 0$, we have $|f(z)| \leq M e^{d|z|}$ for some $d < \pi$. If $f(k) = 0$ for $k = 0, 1, 2, \dots$ then $f(z) = 0$ identically.*

It is illustrative to note that $\sin(\pi z)$ does not satisfy the conditions of the theorem, as it grows like $e^{\pi \operatorname{Im} z}$ on the imaginary axis. On the other hand, the conditions for

n	$s = 2$	$s = 4$	$s = 6$	$s = 8$	$s = 10$	[48]
2	2	6	20	70	252	A000984
3	3	15	93	639	4653	A002893
4	4	28	256	2716	31504	A002895
5	5	45	545	7885	127905	A169714
6	6	66	996	18306	384156	A169715

Table 1: $W_n(s)$ at even integers

Carlson's Theorem are readily verified to hold for $W_n(s)$: the analyticity, as well as exponential growth in the right half-plane, is clear from (11) and because the integral is supported on the finite interval $[0, n]$ only. Likewise, the additional growth condition on the imaginary axis holds: in fact, for fixed real x and varying real y , the absolute value of the moments $|W_n(x + iy)|$ takes its maximal value when $y = 0$. As a consequence, the values $W_n(1), W_n(2), \dots$ determine the distribution of the distance traveled by an n -step walk.

In fact, the even moments $W_n(2k)$ turn out to be right object to look at. Numerical computations or close inspection of the definition (2) reveal that the even moments are given by integer sequences — the square root implicit in (2) disappears when s is even. With this realization one can get started by naively but rapidly computing many values of $W_n(2k)$ as symbolic integrals. Several values are recorded in Table 1.

For small values of n one quickly identifies the resulting integer sequences $f_n(k) := W_n(2k)$ by a lookup in the OEIS [48]. For instance, one observes $W_2(2k) = \binom{2k}{k}$. Indeed,

$$W_2(s) = \binom{s}{s/2} \tag{12}$$

for s not an odd negative integer. This follows readily from (2).

Armed with such observations, one is lead [11] to the combinatorial evaluation

$$W_n(2k) = \sum_{a_1 + \dots + a_n = k} \binom{k}{a_1, \dots, a_n}^2 \tag{13}$$

for integers $k \geq 0$. Combinatorially, this means that the even moment $W_n(2k)$ counts the number of n -letter *abelian squares* of length $2k$ (that is strings xx' of length $2k$ from an alphabet with n letters such that x' is a permutation of x). These numbers have been recently studied for instance by Shallit and Richmond in [41] who obtained their asymptotics.

From this interpretation one readily deduces that the even moments satisfy the convolution identity

$$W_{n_1+n_2}(2k) = \sum_{j=0}^k \binom{k}{j}^2 W_{n_1}(2j)W_{n_2}(2k-2j). \quad (14)$$

Moreover, the form of the evaluation (13) promises that, for fixed n , the even moments $W_n(2k)$ satisfy a linear recurrence with polynomial coefficients. For instance, for $n = 3$,

$$(k+2)^2 W_3(2k+4) - (10k^2 + 30k + 23)W_3(2k+2) + 9(k+1)^2 W_3(2k) = 0.$$

In the light of Carlson's Theorem 2.1, these even moment recurrences can be extended into complex functional equations such as

$$(s+4)^2 W_3(s+4) - 2(5s^2 + 30s + 46)W_3(s+2) + 9(s+2)^2 W_3(s) = 0. \quad (15)$$

These functional equations give meromorphic continuations of the moments to the full complex plane, with poles at certain negative integers. This is illustrated in Figure 2 on the real line and later in Figure 3 on the complex plane. Notice that both $W_3(s)$ and $W_4(s)$ do not have zeroes for negative odd integers; however, as shown in [15], $W_3(-2k-1)$ decays to 0 very rapidly as $k \rightarrow \infty$.

For instance, in the case $n = 3$ one finds that $W_3(s)$ has a simple pole at -2 with residue $\frac{2}{\sqrt{3}\pi}$ and other simple poles at $-2k$ with residues a rational multiple of the one at -2 . More precisely, as found in [14], the pole at $-2k-2$ has residue

$$\text{Res}_{-2k-2}(W_3) = \frac{2}{\pi\sqrt{3}} \frac{W_3(2k)}{3^{2k}} > 0. \quad (16)$$

Similar to (15), for $n = 4$ the functional equation is

$$(s+4)^3 W_4(s+4) - 4(s+3)(5s^2 + 30s + 48)W_4(s+2) + 64(s+2)^3 W_4(s) = 0 \quad (17)$$

and the poles, which are of second order, are again located at the negative even integers. In the case $n = 5$, the functional equation is

$$(s+6)^4 W_5(s+6) - (35(s+5)^4 + 42(s+5)^2 + 3)W_5(s+4) + (s+4)^2(259(s+4)^2 + 104)W_5(s+2) = 225(s+4)^2(s+2)^2 W_5(s). \quad (18)$$

Since

$$\lim_{s \rightarrow -2} (s+2)^2 W_5(s) = \frac{4}{225} (285W_5(0) - 201W_5(2) + 16W_5(4)) = 0,$$

$$\lim_{s \rightarrow -4} (s+4)^2 W_5(s) = -\frac{4}{225} (5W_5(0) - W_5(2)) = 0,$$

the first two poles — and hence all — are simple. In general, it is conjectured (and verified for $n \leq 45$) in [14] that, for odd n , all poles of $W_n(s)$ are simple; double poles are only expected when $4|n$.

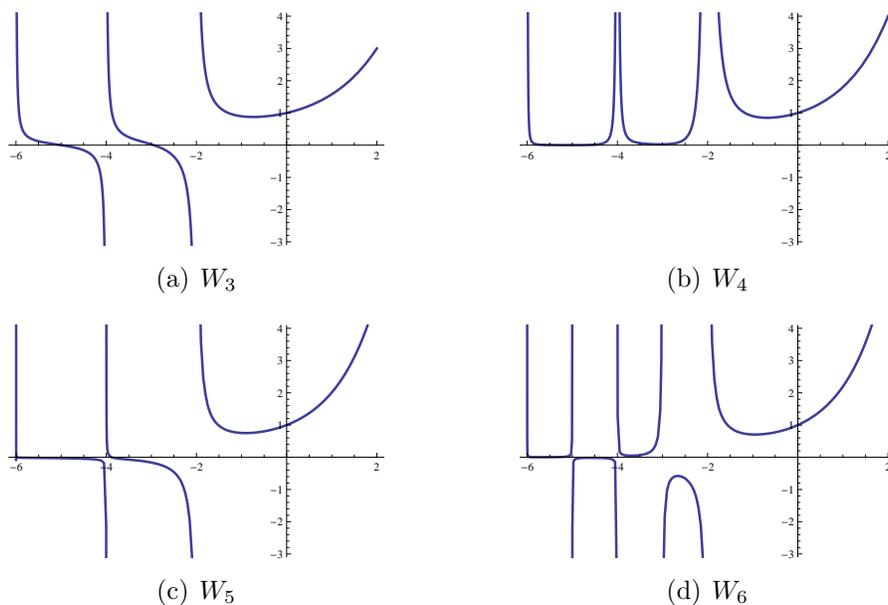


Figure 2: Various W_n and their analytic continuations

2.2 Evaluations of the first moments for $n = 3, 4$

It is well-known and follows directly from (12) that the average distance traveled by a random walk in two steps is $W_2(1) = \frac{4}{\pi} \approx 1.27324$. In this section we are concerned with similar evaluations for the average distance traveled in more than two steps. In [11], our initial interest was fueled by the following observation: from (13) we have

that

$$W_3(2k) = \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j} = {}_3F_2 \left(\begin{matrix} \frac{1}{2}, -k, -k \\ 1, 1 \end{matrix} \middle| 4 \right) \quad (19)$$

for integers $k \geq 0$. Numerical experimentation, however, suggested that

$$W_3(k) = \operatorname{Re} {}_3F_2 \left(\begin{matrix} \frac{1}{2}, -\frac{k}{2}, -\frac{k}{2} \\ 1, 1 \end{matrix} \middle| 4 \right) \quad (20)$$

whenever k is a nonnegative integer. After confirming (20) in the case $k = 1$ to more than 175 digits, this was shown in [11] to indeed hold true. As a consequence a closed formula was found for $W_3(1) \approx 1.57460$. In the sequel we will sketch a different route to this evaluation which will be given in (27).

The *Meijer G-function*, introduced in 1936 by the Dutch mathematician Cornelis Simon Meijer (1904-1974), is a broad generalization of hypergeometric functions — capturing Bessel Y , K and many other special functions. As such it is important in computer algebra systems — if better hidden. The Meijer G -function is defined [1], for parameter vectors \mathbf{a} and \mathbf{b} , by

$$\begin{aligned} G_{p,q}^{m,n} \left(\begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \middle| x \right) &= G_{p,q}^{m,n} \left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \middle| x \right) \\ &= \frac{1}{2\pi i} \int_L \frac{\prod_{k=1}^m \Gamma(b_k - t) \prod_{k=1}^n \Gamma(1 - a_k + t)}{\prod_{k=m+1}^q \Gamma(1 - b_k + t) \prod_{k=n+1}^p \Gamma(a_k - t)} x^t dt. \end{aligned} \quad (21)$$

In the case $|x| < 1$ and $p = q$, the contour L is a loop that starts at infinity on a line parallel to the positive real axis, encircles the poles of the $\Gamma(b_k - t)$ once in the negative sense and returns to infinity on another line parallel to the positive real axis. L is a similar contour when $|x| > 1$. By Slater's Theorem [34, p. 57], a Meijer G -function frequently may be expressed as a superposition of generalized hypergeometric functions.

As first observed by Crandall [21] using *Mathematica*, we have the Meijer G -function representations

$$W_3(s) = \frac{\Gamma(1 + s/2)}{\Gamma(1/2)\Gamma(-s/2)} G_{3,3}^{2,1} \left(\begin{matrix} 1, 1, 1 \\ 1/2, -s/2, -s/2 \end{matrix} \middle| \frac{1}{4} \right), \quad (22)$$

$$W_4(s) = \frac{2^s \Gamma(1 + s/2)}{\pi \Gamma(-s/2)} G_{4,4}^{2,2} \left(\begin{matrix} 1, (1-s)/2, 1, 1 \\ 1/2, -s/2, -s/2, -s/2 \end{matrix} \middle| 1 \right), \quad (23)$$

valid whenever s is not an odd integer. In the case of W_4 , we further require $\text{Re } s > -2$. Both representations may be proven using Mellin calculus, see [14]. By Slater's theorem, the respective Meijer G -functions can be expanded in terms of generalized hypergeometric functions as

$$W_3(s) = \frac{1}{2^{2s+1}} \tan\left(\frac{\pi s}{2}\right) \left(\frac{s}{s-1}\right)^2 {}_3F_2\left(\frac{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}}{\frac{s+3}{2}, \frac{s+3}{2}} \middle| \frac{1}{4}\right) + \left(\frac{s}{s/2}\right) {}_3F_2\left(\frac{-\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2}}{1, -\frac{s-1}{2}} \middle| \frac{1}{4}\right), \quad (24)$$

$$W_4(s) = \frac{1}{2^{2s}} \tan\left(\frac{\pi s}{2}\right) \left(\frac{s}{s-1}\right)^3 {}_4F_3\left(\frac{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{s}{2} + 1}{\frac{s+3}{2}, \frac{s+3}{2}, \frac{s+3}{2}} \middle| 1\right) + \left(\frac{s}{s/2}\right) {}_4F_3\left(\frac{\frac{1}{2}, -\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2}}{1, 1, -\frac{s-1}{2}} \middle| 1\right) \quad (25)$$

with the previous restrictions on s . While these representations are not immediately helpful in the case of $W_3(1)$ and $W_4(1)$, they enable us, coupled with the functional equations (15) and (17), to plot the moments in the complex plane using a computer algebra system such as *Mathematica*: in Figure 3 each complex value is colored differently with black indicating a zero and white a pole.

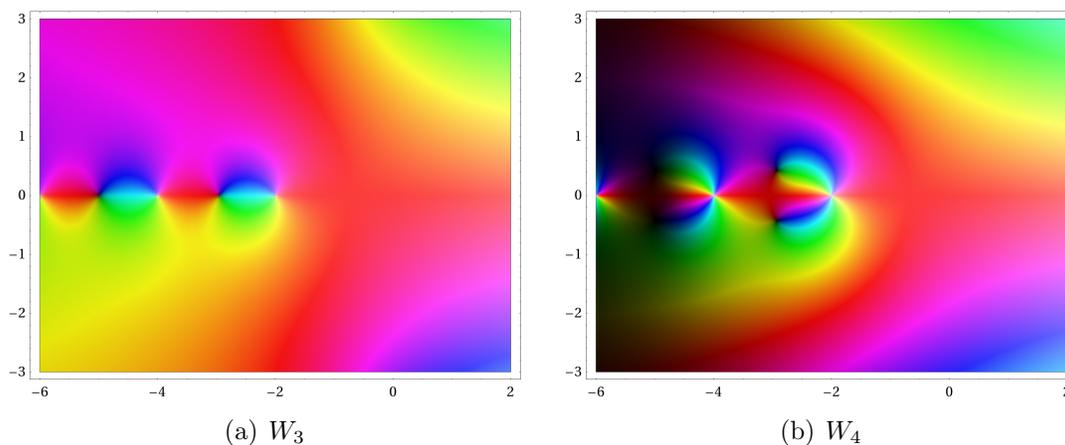


Figure 3: W_3 and W_4 in the complex plane

In the case $n = 3$ a more tractable hypergeometric representation can be given. Starting with a Bessel integral representation valid for even moments and applying Carlson's Theorem, it is deduced in [15] that, for s not a negative integer < -1 ,

$$W_3(s) = \frac{3^{s+3/2}}{2\pi} \frac{\Gamma(1+s/2)^2}{\Gamma(s+2)} {}_3F_2\left(\frac{\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2}}{1, \frac{s+3}{2}} \middle| \frac{1}{4}\right). \quad (26)$$

From here, aided by a computer algebra system such as *Maple* or knowledge of elliptic integral identities, one finds that

$$W_3(-1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right), \quad (27)$$

$$\begin{aligned} W_3(1) &= W_3(-1) + \frac{6}{\pi^2} \frac{1}{W_3(-1)} \\ &= \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4} \frac{2^{2/3}}{\pi^4} \Gamma^6\left(\frac{2}{3}\right). \end{aligned} \quad (28)$$

This closed formula for the average distance traveled by a random walk in three steps was originally proven in [11] by first establishing the experimentally found (20) and then applying Legendre's identity as well as singular values of elliptic integrals [7].

Using the Meijer G -function representation of W_4 , it is shown in [14] by combining several transformations for Meijer G - and hypergeometric functions that

$$\begin{aligned} W_4(-1) &= \frac{\pi}{4} {}_7F_6\left(\begin{matrix} \frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{1}{4}, 1, 1, 1, 1, 1 \end{matrix} \middle| 1\right) \\ &= \frac{\pi}{4} {}_6F_5\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1, 1, 1 \end{matrix} \middle| 1\right) + \frac{\pi}{64} {}_6F_5\left(\begin{matrix} \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \\ 2, 2, 2, 2, 2 \end{matrix} \middle| 1\right) \\ &= \frac{\pi}{4} \sum_{n=0}^{\infty} \frac{(4n+1) \binom{2n}{n}^6}{4^{6n}}. \end{aligned} \quad (29)$$

More work shows that $W_4(1)$ evaluates in similar terms as

$$W_4(1) = \frac{3\pi}{4} {}_7F_6\left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 1, 1 \end{matrix} \middle| 1\right) - \frac{3\pi}{8} {}_7F_6\left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 2, 1 \end{matrix} \middle| 1\right). \quad (30)$$

Again, each ${}_7F_6$ term may be written as a combination of two ${}_6F_5$'s.

For five-step walks things become much more difficult. We do not know if it is possible to give a (hyper-)closed form for $W_5(\pm 1)$ (a general one-dimensional integral representation for $W_n(\pm 1)$ is recorded in (57)). Nonetheless, the residues of W_5 turn out to be expressible in closed form — this is sketched in Section 2.5.

2.3 Densities of random walks

Next, we turn our attention to the probability densities p_n related to the moments by (11). For these densities Kluyver [30] derived the Bessel integral representation

$$p_n(x) = \int_0^\infty xt J_0(xt) J_0^n(t) dt, \quad (31)$$

where J_n denotes the Bessel function of the first kind. Similarly, the cumulative density function P_n can be expressed as

$$P_n(x) = \int_0^\infty x J_1(xt) J_0^n(t) dt. \quad (32)$$

Curiously, the analogous integrand functions for random walks in three dimensions are elementary, [51, §13.49]. We further remark that, from (32),

$$P_n(1) = \frac{J_0(0)^{n+1}}{n+1} = \frac{1}{n+1}. \quad (33)$$

In other words, the probability that a random walk is within one unit from its origin after n steps is $\frac{1}{n+1}$. A remarkably short proof of this classical result has recently been given by Bernardi in [3].

It is visually clear from the graphs in Figure 1 that p_n is getting smoother for increasing n . More precisely, it follows from (31), on using the asymptotic formula for J_0 for large arguments and dominated convergence, that p_{n+4} is $\lfloor n/2 \rfloor$ times continuously differentiable.

Many properties of the densities $p_n(x)$ can be obtained from corresponding properties of the moments $W_n(s)$ by virtue of their relation (11), by which p_n is the inverse Mellin transform of $W_n(s-1)$. Recall that if $F(s) = \mathcal{M}[f; s]$ is the Mellin transform of $f(x)$ then in the appropriate strips of convergence

- $\mathcal{M}[x^\mu f(x); s] = F(s + \mu)$,
- $\mathcal{M}[D_x f(x); s] = -(s-1)F(s-1)$.

It follows that the functional equations for the moments $W_n(s)$ translate into differential equations for the densities $p_n(x)$. For instance in the case $n=4$, the functional equation (17) formally produces the differential equation $A_4 \cdot p_4(x) = 0$, where A_4 is the operator

$$A_4 = x^4(\theta+1)^3 - 4x^2\theta(5\theta^2+3) + 64(\theta-1)^3, \quad (34)$$

and $\theta = xD_x$. However, it should be noted that care [15] is needed when rigorously establishing that the densities p_n satisfy the formally obtained differential equations: for instance, $p_4(x)$ is approximated by a constant multiple of $\sqrt{4-x}$ as $x \rightarrow 4^-$, so that the second derivative of p_4 is not even locally integrable. In particular, p_4'' does not have a Mellin transform in the classical sense.

In general, it is shown in [15] that the density p_n satisfies a Fuchsian differential equation of order $n - 1$. From the leading coefficient of this differential equation one finds that p_n is real analytic except at 0 and the positive integers $n, n - 2, n - 4, \dots$.

Knowledge of the pole structure of the moments $W_n(s)$, as briefly discussed in Section 2.1, also transfers profitably to the densities $p_n(x)$: as a general principle, [28, Appendix B.7], the asymptotic behaviour of a function at zero is determined by the poles of its Mellin transform which lie to the left of the fundamental strip. From the fact that the poles of $W_n(s)$ occur at specific negative integers and are at most of second order, it then follows that p_n has a local expansion at 0 as a power series with additional logarithmic terms in the presence of double poles.

2.4 The densities p_3 and p_4

To illustrate this point, we first consider the case of p_3 , which is depicted in Figure 1(a). Since the poles of $W_3(s)$ are simple, the explicit knowledge (16) of the residues implies that

$$p_3(x) = \frac{2x}{\pi\sqrt{3}} \sum_{k=0}^{\infty} W_3(2k) \left(\frac{x}{3}\right)^{2k}, \quad (35)$$

which is valid for $0 \leq x \leq 1$. Surprisingly, as found numerically in [14], the density p_3 satisfies the functional equation

$$p_3(x) = \frac{4x}{(3-x)(x+1)} p_3\left(\frac{3-x}{1+x}\right). \quad (36)$$

Note that $x \mapsto \frac{3-x}{1+x}$ is an involution on $[0, 3]$ sending $[0, 1]$ to $[1, 3]$. Equation (36) together with (35) thus makes apparent the behaviour of p_3 at 3; for instance, it implies that

$$p_3(3) = \frac{3}{4} p_3'(0) = \frac{\sqrt{3}}{2\pi}.$$

Indeed, a single easily computed hypergeometric expression can be given for p_3 :

$$p_3(x) = \frac{2\sqrt{3}x}{\pi(3+x^2)} {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; \frac{x^2(9-x^2)^2}{(3+x^2)^3}\right). \quad (37)$$

In terms of the cubically convergent mean iteration $\text{AG}_3(a, b)$, studied in [6] and defined as the limit of iterating

$$a_{n+1} = \frac{a_n + 2b_n}{3}, \quad b_{n+1} = \sqrt[3]{b_n \left(\frac{a_n^2 + a_n b_n + b_n^2}{3}\right)},$$

beginning with $a_0 = a$ and $b_0 = b$, this may also be expressed as

$$p_3(x) = \frac{2\sqrt{3}}{\pi} \frac{x}{\text{AG}_3(3 + x^2, 3 | 1 - x^2|^{2/3})}. \quad (38)$$

Thus, we have remedied the problems with the century-old equation (10).

The “shark-fin” density p_4 , shown in Figure 1(b), turns out to be amenable to similar considerations. In [15] it is ultimately deduced that, on $2 \leq x \leq 4$,

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16 - x^2}}{x} {}_3F_2 \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{(16 - x^2)^3}{108x^4} \right). \quad (39)$$

Once discovered — as it was by large-scale symbolic experimentation — this identity may be proven automatically from (34) after somewhat tediously establishing the first three terms of the expansion of $p_4(x)$ as $x \rightarrow 4^-$. The hypergeometric representation (39) proves, for instance, that

$$p_4(2) = \frac{2^{7/3}\pi}{3\sqrt{3}} \Gamma\left(\frac{2}{3}\right)^{-6} = \frac{\sqrt{3}}{\pi} W_3(-1). \quad (40)$$

Marvelously, we first found and later proved that, on *all* of $0 \leq x \leq 4$,

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16 - x^2}}{x} \text{Re} {}_3F_2 \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{(16 - x^2)^3}{108x^4} \right). \quad (41)$$

Observe how, on $0 < x < 2$, taking the real part of an analytically continued ${}_3F_2$ masks the fact that the expansion of p_4 at 0 involves logarithmic terms:

$$p_4(x) = -\frac{3}{2\pi^2} x \log(x) + \frac{9}{2\pi^2} \log(2)x + O(x^3).$$

2.5 The density p_5

In the case of p_5 our knowledge is less complete. From the general Mellin calculus described in the context of (34), it follows that the density p_5 is real analytic on $(0, 5)$ except at 1 and 3, and satisfies the differential equation $A_5 \cdot p_5(x) = 0$, where A_5 is the operator

$$A_5 = x^6(\theta + 1)^4 - x^4(35\theta^4 + 42\theta^2 + 3) + x^2(259(\theta - 1)^4 + 104(\theta - 1)^2) - (15(\theta - 3)(\theta - 1))^2 \quad (42)$$

and $\theta = xD_x$. As in the case of p_3 , it follows from the simplicity of the poles of W_5 that p_5 has a power series expansion at 0 with the coefficients determined by the residues of W_5 :

$$p_5(x) = \sum_{k=0}^{\infty} r_{5,k} x^{2k+1} \quad (43)$$

where $r_{5,k} = \text{Res}_{-2k-2} W_5$. The residues $r_{5,k}$, by the functional equation (18) for W_5 , satisfy the recursive relation

$$\begin{aligned} (15(2k+2)(2k+4))^2 r_{5,k+2} &= (259(2k+2)^4 + 104(2k+2)^2) r_{5,k+1} \\ &- (35(2k+1)^4 + 42(2k+1)^2 + 3) r_{5,k} + (2k)^4 r_{5,k-1} \end{aligned} \quad (44)$$

with initial values $r_{5,-1} = 0$ and $r_{5,0}, r_{5,1}$. A surprising bonus of the evaluation of p_4 is that these initial values can be made explicit:

$$r_{5,0} = p_4(1) = \frac{\sqrt{5}}{40} \frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{\pi^4}. \quad (45)$$

This is deduced in [15] and makes use of the general fact that, when $n \geq 4$, $\text{Res}_{-2} W_{n+1} = p_n(1)$, which is a consequence of (54). Numerical computations based on the residue evaluations of (49) and (50) of Section 2.6, led us to conjecture — and verify to 500 digits — that the residue of W_5 at -4 has a similar closed form:

$$r_{5,1} \stackrel{?}{=} \frac{13}{225} r_{5,0} - \frac{2}{5\pi^4} \frac{1}{r_{5,0}}. \quad (46)$$

Hence, by (44), all residues of W_5 are analogous combinations. Computer algebra programs do not seem able to shed much light on the form of the solutions to (42) or of (44). Nonetheless, we still hope to find some closed form for p_5 .

By computing the first four residues, we find

$$p_5(x) = 0.329934x + 0.00661673x^3 + 0.000262333x^5 + 0.0000141185x^7 + O(x^9)$$

near 0 which explains the strikingly straight shape of $p_5(x)$ on $[0, 1]$, visible in Figure 1(c).

This phenomenon was observed by Pearson [39], who stated that for $p_5(x)/x$ between $x = 0$ and $x = 1$,

“the graphical construction, however carefully reinvestigated, did not permit of our considering the curve to be anything but a *straight* line. . . Even if it is not absolutely true, it exemplifies the extraordinary power of such integrals of J products [that is, (31)] to give extremely close approximations to such simple forms as horizontal lines.”

This conjecture was investigated in detail in [26] wherein the nonlinearity was first rigorously established. This work and various more recent papers, especially [2], highlight the continuing difficulty of computing the underlying Bessel integrals. Interestingly, Sidi's methods [45, 46] proved useful only for a product of an odd number of Bessel functions. Subsequent to the work in [2], Sidi has however proposed an enhanced method [47]. We have not yet had a chance to test it to extreme precision.

2.6 Derivative evaluations of the moments

As illustrated in the previous section, the residues of $W_n(s)$ are very important for studying the densities p_n as they directly translate into behaviour of p_n at 0. Using the functional equation for $W_n(s)$ and L'Hôpital's rule, the residues may be expressed as linear combinations of derivatives of W_n at even integers. For instance,

$$\text{Res}_{-2}(W_3) = \frac{8 + 12W_3'(0) - 4W_3'(2)}{9}, \quad (47)$$

$$\text{Res}_{-2}(W_4) = \frac{9 + 18W_4'(0) - 3W_4'(2) + 4W_4''(0) - W_4''(2)}{16}, \quad (48)$$

$$\text{Res}_{-2}(W_5) = \frac{16 + 1140W_5'(0) - 804W_5'(2) + 64W_5'(4)}{225}, \quad (49)$$

$$\text{Res}_{-4}(W_5) = \frac{26 \text{Res}_{-2}(W_5) - 16 - 20W_5'(0) + 4W_5'(2)}{225}. \quad (50)$$

The derivatives of moments are therefore discussed in [15]. In particular, differentiating the hypergeometric expressions (24), (25) for W_3 and W_4 , it is deduced that

$$W_3'(0) = \frac{1}{\pi} {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| \frac{1}{4} \right) = \frac{1}{\pi} \text{Cl}_2 \left(\frac{\pi}{3} \right), \quad (51)$$

$$W_4'(0) = \frac{4}{\pi^2} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1 \\ \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1 \right) = \frac{7\zeta(3)}{2\pi^2}. \quad (52)$$

Note that the first identity uses

$$2 \sin(\theta) {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| \sin^2 \theta \right) = \text{Cl}_2(2\theta) + 2\theta \log(2 \sin \theta) \quad (53)$$

with $\theta = \pi/6$, while the second identity is elementary. Equation (53) is machine provable once found. Depending on the computer algebra system used, one may or not be able to sum these directly. For example, in *Mathematica 7* the input

`HypergeometricPFQ[{1/2,1/2,1/2,1}, {3/2,3/2,3/2}, 1]`

is immediately evaluated as $\frac{7}{8}\zeta(3)$. *Maple 15* does not evaluate the hypergeometric series symbolically. Still, the evaluation (52) can be discovered numerically: the code

```
H := hypergeom( [1/2,1/2,1/2,1], [3/2,3/2,3/2], 1 );
identify( evalf(H) );
```

returns $\frac{7}{8}\zeta(3)$. Both *Mathematica 8* and *Maple 15* fail to resolve the hypergeometric series in (51).

As indicated in the introduction, the derivatives of the moments at zero are (logarithmic) Mahler measures (3). In particular, $W'_3(0) = \mu(1+x+y)$ and $W'_4(0) = \mu(1+x+y+z)$. The respective evaluations above are thus rediscoveries of the Mahler measure evaluations due to C. Smyth [42, (1.1) and (1.2)] with proofs first published in [16, Appendix 1].

A general integral representation for $W'_n(0)$ may be deduced from

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1 + \frac{s}{2})}{\Gamma(k - \frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x} \frac{d}{dx} \right)^k J_0^n(x) dx, \quad (54)$$

which is valid for $2k > s > -\frac{n}{2}$. Equation (54) was first obtained by Broadhurst [18] from (31) and is further discussed in [14]. It implies, for instance, that

$$W'_n(0) = \log(2) - \gamma - \int_0^1 (J_0^n(x) - 1) \frac{dx}{x} - \int_1^\infty J_0^n(x) \frac{dx}{x} \quad (55)$$

$$= \log(2) - \gamma - n \int_0^\infty \log(x) J_0^{n-1}(x) J_1(x) dx. \quad (56)$$

Numerical computation of these derivatives is discussed in detail in [2]. Equation (54) is also a very useful oscillatory one-dimensional representation of the moments $W_n(s)$. In particular, it allows us to write

$$W_n(-1) = \int_0^\infty J_0^n(x) dx, \quad (57a)$$

$$W_n(1) = n \int_0^\infty J_1(x) J_0(x)^{n-1} \frac{dx}{x}. \quad (57b)$$

3 Multiple Mahler measures

Beyond the comparably simple evaluation of the Mahler measures $\mu(1+x+y)$ and $\mu(1+x+y+z)$ due to Smyth and reobtained in Section 2.6, there exist many

more Mahler measures which evaluate in terms of L -series. A very pleasant survey containing a host of examples is [17]. In many cases, however, these evaluations are only known conjecturally. A recent success was the proof by Rogers and Zudilin [43] that

$$\mu\left(1+x+y+\frac{1}{x}+\frac{1}{y}\right)=L'_E(0)=\frac{15}{4\pi^2}L_E(2), \quad (58)$$

which was conjectured by Boyd, based on a result of Deninger [25] that implies (58) up to a rational constant. Here, L_E is the L -series associated to an elliptic curve E with conductor 15.

We consider again the Mahler measures $\mu(1+x_1+\dots+x_{n-1})=W'_n(0)$ which we encountered as derivative values of moments of random walks. Before taking a second look at the classical cases $n=3$ and $n=4$, we remark that, at least conjecturally, evaluations in terms of L -series are also known for $n=5$ and $n=6$:

$$W'_5(0)\stackrel{?}{=} -L'_f(-1)=\frac{675\sqrt{15}}{16\pi^5}L_f(4), \quad (59)$$

$$W'_6(0)\stackrel{?}{=} -8L'_g(-1)=\frac{648}{\pi^6}L_g(5). \quad (60)$$

Here, f, g are certain cusp forms, defined in [27] where both conjectural identities are attributed to Rodriguez-Villegas. Numerical confirmation to 600 and to 80 digits respectively is detailed in [2]. The difference in our level of numerical confirmation is explained by the already mentioned failure of Sidi's method [46] for $n=6$.

Stepping back to the much simpler cases of $n=3$ and 4, we recall *Jensen's formula*

$$\int_0^1 \log|\alpha+e^{2\pi it}| dt = \log(\max\{|\alpha|, 1\}), \quad (61)$$

and apply it to reduce $\mu(1+x+y)$ to a one-dimensional integral:

$$\mu(1+x+y) = \int_{1/6}^{5/6} \log(2\sin(\pi y)) dy = \frac{1}{\pi} \text{Ls}_2\left(\frac{\pi}{3}\right) = \frac{1}{\pi} \text{Cl}_2\left(\frac{\pi}{3}\right). \quad (62)$$

The result, of course, agrees with (51).

To similarly evaluate $\mu(1+x+y+z)$, we follow Boyd [16, Appendix 1] and observe, on applying Jensen's formula, that for complex constants a and b

$$\mu(ax+b) = \log|a| \vee \log|b|. \quad (63)$$

Writing $w = y/z$, we once more reobtain [12] Smyth's result (52):

$$\begin{aligned}
\mu(1+x+y+z) &= \mu(1+x+z(1+w)) = \mu(\log|1+w| \vee \log|1+x|) \\
&= \frac{1}{\pi^2} \int_0^\pi d\theta \int_0^\pi \max \left\{ \log \left(2 \sin \frac{\theta}{2} \right), \log \left(2 \sin \frac{t}{2} \right) \right\} dt \\
&= \frac{2}{\pi^2} \int_0^\pi d\theta \int_0^\theta \log \left(2 \sin \frac{\theta}{2} \right) dt \\
&= \frac{2}{\pi^2} \int_0^\pi \theta \log \left(2 \sin \frac{\theta}{2} \right) d\theta \\
&= -\frac{2}{\pi^2} \text{Ls}_3^{(1)}(\pi) = \frac{7}{2} \frac{\zeta(3)}{\pi^2}. \tag{64}
\end{aligned}$$

For another example illustrating the utility of log-sine integrals to evaluate multiple Mahler measures we consider

$$\mu_c := \mu(y^2(x+1)^2 + y(x^2 + 2cx + 1) + (x+1)^2). \tag{65}$$

The following evaluations were conjectured by Boyd in 1998 and first proven in [50] using *Bloch-Wigner* logarithms:

$$\mu_3 = \frac{16}{3\pi} L_{-4}(2) = \frac{16}{3\pi} G, \tag{66}$$

$$\mu_{-5} = \frac{5\sqrt{3}}{\pi} L_{-3}(2) = \frac{20}{3\pi} \text{Cl}_2\left(\frac{\pi}{3}\right), \tag{67}$$

where L_{-n} denotes a primitive L -series and G is Catalan's constant. Using a variant of Jensen's formula and slick trigonometry [4], one arrives at

$$\begin{aligned}
\mu_3 &= \frac{1}{\pi} \int_0^\pi \log(1 + 4|\cos \theta| + 4|\cos^2 \theta|) d\theta \\
&= \frac{4}{\pi} \int_0^{\pi/2} \log(1 + 2\cos \theta) d\theta \\
&= \frac{4}{\pi} \int_0^{\pi/2} \log \left(\frac{2 \sin \frac{3\theta}{2}}{2 \sin \frac{\theta}{2}} \right) d\theta \\
&= \frac{4}{3\pi} \left(\text{Ls}_2 \left(\frac{3\pi}{2} \right) - 3 \text{Ls}_2 \left(\frac{\pi}{2} \right) \right) \\
&= \frac{16}{3} \frac{L_{-4}(2)}{\pi}
\end{aligned}$$

as claimed, since $\text{Ls}_2\left(\frac{3\pi}{2}\right) = -\text{Ls}_2\left(\frac{\pi}{2}\right) = \text{L}_{-4}(2)$, which is Catalan's constant G . Much the same techniques work for μ_{-5} . Additionally, there is one bonus case:

$$\mu_{-1} = \frac{1}{\pi} \left\{ \frac{1}{2} B\left(\frac{1}{4}, \frac{1}{4}\right) {}_3F_2\left(\frac{1}{4}, \frac{1}{4}, 1 \middle| \frac{1}{4}\right) - \frac{1}{6} B\left(\frac{3}{4}, \frac{3}{4}\right) {}_3F_2\left(\frac{3}{4}, \frac{3}{4}, 1 \middle| \frac{1}{4}\right) \right\}. \quad (68)$$

Returning to the multiple Mahler measure

$$\mu_k(1+x+y_*) := \mu(1+x+y_1, 1+x+y_2, \dots, 1+x+y_k), \quad (69)$$

as defined in (5) in the introduction, we see that it can be put in the form

$$\mu_k(1+x+y_*) = \int_{1/6}^{5/6} \log^k |1 - e^{2\pi i t}| dt \quad (70)$$

upon using Jensen's formula (61). This was used by Sasaki [44] to deduce the evaluation $\mu_2(1+x+y_*) = \frac{\pi^2}{54}$. More generally, as shown in [12], immediately from (70) and the definition (6) of the log-sine integrals, we have

$$\mu_k(1+x+y_*) = \frac{1}{\pi} \text{Ls}_{k+1}\left(\frac{\pi}{3}\right) - \frac{1}{\pi} \text{Ls}_{k+1}(\pi) \quad (71)$$

as indicated in (7). We give explicit evaluations for the involved log-sine integrals in (73) and (82).

More examples of multiple Mahler measures that allow convenient evaluation in terms of log-sine integrals are contained in [12]. This was one of the motivations for a systematic study of log-sine integrals detailed in [13] and sketched next in Section 4.

4 Log-sine integrals

In this section we consider evaluations of the log-sine integrals introduced in (6). Our emphasis is on automatically provable evaluations. We will only sketch the ideas of such evaluations — details may be found in [13].

An easy initial and motivating example is the well-known exponential generating function, [32, 33],

$$-\frac{1}{\pi} \sum_{m=0}^{\infty} \text{Ls}_{m+1}(\pi) \frac{\lambda^m}{m!} = \frac{\Gamma(1+\lambda)}{\Gamma^2\left(1+\frac{\lambda}{2}\right)} = \binom{\lambda}{\lambda/2}. \quad (72)$$

Besides its surprising simplicity and relation with moments of walks considered in Section 2 via $W_2(s) = \binom{s}{s/2}$, it provides a convenient way to evaluate basic log-sine integrals at π using a computer algebra system.

For instance, in *Maple* the code

for k from 2 to 8 do
simplify(subs(x=0,diff(Pi*binomial(x,x/2),x\$k))) od
automatically produces the evaluations:

$$\text{Ls}_2(\pi) = 0, \quad (73a)$$

$$-\text{Ls}_3(\pi) = \frac{1}{12} \pi^3, \quad (73b)$$

$$\text{Ls}_4(\pi) = \frac{3}{2} \pi \zeta(3), \quad (73c)$$

$$-\text{Ls}_5(\pi) = \frac{19}{240} \pi^5, \quad (73d)$$

$$\text{Ls}_6(\pi) = \frac{45}{2} \pi \zeta(5) + \frac{5}{4} \pi^3 \zeta(3), \quad (73e)$$

$$-\text{Ls}_7(\pi) = \frac{275}{1344} \pi^7 + \frac{45}{2} \pi \zeta(3)^2, \quad (73f)$$

$$\text{Ls}_8(\pi) = \frac{2835}{4} \pi \zeta(7) + \frac{315}{8} \pi^3 \zeta(5) + \frac{133}{32} \pi^5 \zeta(3). \quad (73g)$$

Of course, a more efficient way to automatically obtain these evaluations is to rewrite the generating function (72) as a recurrence equation.

Remark 4.1. By combining (4) and (12) with (72), one notes that

$$\mu_k(1+x) = -\frac{1}{\pi} \text{Ls}_{k+1}(\pi). \quad (74)$$

This Mahler measure is evaluated in [31, Theorem 3] as

$$\mu_k(1+x) = (-1)^k k! \sum_{n=1}^{\infty} \frac{1}{4^n} \sum_{b_j \geq 2, \sum b_j = k} \zeta(b_1, b_2, \dots, b_n), \quad (75)$$

and the right-hand side is used in [31, Example 5] to derive values for $\mu_k(1+x)$ when $k \leq 6$. In light of (74), these are equivalent to the respective evaluations in (73). \diamond

Log-sine integrals at 2π also evaluate in terms of zeta values only. This is a consequence of the following generating function observed by Lewin [33, 7.9.8]:

$$-\sum_{n,k \geq 0} \text{Ls}_{n+k+1}^{(k)}(2\pi) \frac{\lambda^n}{n!} \frac{(i\mu)^k}{k!} = \int_0^{2\pi} \left(2 \sin \frac{\theta}{2}\right)^\lambda e^{i\mu\theta} d\theta = 2\pi e^{i\mu\pi} \left(\frac{\lambda}{2} + \mu\right). \quad (76)$$

As just illustrated for basic log-sine integrals at π this allows for an automatic treatment of log-sine integrals at 2π .

Remark 4.2. Many explicit evaluations of $\text{Ls}_n^{(k)}(2\pi)$ for $k = 1, 2, \dots, 6$ are given in [20], though almost half of them are stated incorrectly: for $k = 1$ and $n = 10, 11, 12$, for $k = 2$ and $n = 9, 11, 12, 13$, for $k = 3$ and $n = 12, 13, 14$, for $k = 4$ and $n = 8, 10, 12, 13, 14, 15$, for $k = 5$ and $n = 10, 13, 14, 15, 16$, as well as for $k = 6$ and $n = 8, 10, 11, 12$ the formulae need correction. For each k we record the corrected value of $\text{Ls}_n^{(k)}(2\pi)$ with n minimal for which this is necessary:

$$-\text{Ls}_{10}^{(1)}(2\pi) = \frac{11813\pi^{10}}{5760} + 105\pi^4\zeta(3)^2 + 3780\pi^2\zeta(3)\zeta(5), \quad (77a)$$

$$-\text{Ls}_9^{(2)}(2\pi) = \frac{3517\pi^9}{5040} + 90\pi^3\zeta(3)^2 + 900\pi\zeta(3)\zeta(5), \quad (77b)$$

$$\begin{aligned} -\text{Ls}_{12}^{(3)}(2\pi) &= \frac{39223\pi^{12}}{6336} + 735\pi^6\zeta(3)^2 + 13860\pi^4\zeta(3)\zeta(5) \\ &\quad + 45360\pi^2\zeta(5)^2 + 90720\pi^2\zeta(3)\zeta(7), \end{aligned} \quad (77c)$$

$$-\text{Ls}_8^{(4)}(2\pi) = -20\pi^5\zeta(3) - 84\pi^3\zeta(5) + 360\pi\zeta(7), \quad (77d)$$

$$-\text{Ls}_{10}^{(5)}(2\pi) = \frac{143\pi^{10}}{105} + 600\pi^4\zeta(3)^2 + 1440\pi^2\zeta(3)\zeta(5), \quad (77e)$$

$$-\text{Ls}_8^{(6)}(2\pi) = -192\pi^5\zeta(3) + 960\pi^3\zeta(5) - 1440\pi\zeta(7). \quad (77f)$$

All of these values have been automatically obtained using the routines described and implemented by the authors in [13]. The resulting computer algebra packages can be downloaded from the website of the second author; a link is given in Section 5. To obtain, for instance, the evaluation (77e) in *Mathematica* the following self-explanatory code is sufficient:

```
LsToLi [ -Ls [10, 5, 2Pi] ]
```

This cautionary example underscores the utility of automating the evaluation of log-sine integrals. \diamond

Searching for a way to generalize the generating function approach used in (72) and (76) to general log-sine integrals $\text{Ls}_n^{(k)}(\pi)$ at π , we derived, [13], the generating function

$$-\sum_{n,k \geq 0} \text{Ls}_{n+k+1}^{(k)}(\pi) \frac{\lambda^n (i\mu)^k}{n! k!} = i \sum_{n \geq 0} \binom{\lambda}{n} \frac{(-1)^n e^{i\pi \frac{\lambda}{2}} - e^{i\pi \mu}}{\mu - \frac{\lambda}{2} + n}, \quad (78)$$

valid for $2|\mu| < \lambda < 1$. While the generating function (78) may appear more complicated than (72) or (76), it turns out to be just as suited for the purpose of conveniently extracting coefficients. The required details are described in [13] while we

just demonstrate a few sample evaluations here:

$$\text{LS}_3^{(1)}(\pi) = \frac{7}{4}\zeta(3), \quad (79a)$$

$$\text{LS}_4^{(1)}(\pi) = -2\text{Li}_{3,1}(-1) - \frac{11}{720}\pi^4, \quad (79b)$$

$$\text{LS}_4^{(2)}(\pi) = -\frac{3}{2}\pi\zeta(3), \quad (79c)$$

$$\text{LS}_5^{(1)}(\pi) = 6\text{Li}_{3,1,1}(-1) - \frac{105}{32}\zeta(5) + \frac{1}{4}\pi^2\zeta(3), \quad (79d)$$

$$\text{LS}_5^{(2)}(\pi) = -4\pi\text{Li}_{3,1}(-1) - \frac{1}{120}\pi^5, \quad (79e)$$

$$\text{LS}_5^{(3)}(\pi) = \frac{93}{8}\zeta(5) - \frac{9}{4}\pi^2\zeta(3). \quad (79f)$$

Observe that, in contrast to the case of basic log-sine integrals at π which may be expressed in terms of zeta values only, the evaluation of general log-sine integrals at π additionally requires Nielsen polylogarithms at -1 .

This turns out to be a general fact: the evaluation of the log-sine integral $\text{LS}_n^{(k)}(\tau)$ can be done in terms of Nielsen polylogarithms with argument $e^{i\tau}$, which split into Clausen and Glaisher functions at τ according to (8) and (9). More specifically, the following reduction formula, valid for $0 \leq \tau \leq 2\pi$ and $n - k \geq 2$, is derived in [13]:

$$\begin{aligned} \zeta(k, \{1\}^n) &= \sum_{j=0}^{k-2} \frac{(-i\tau)^j}{j!} \text{Li}_{k-j, \{1\}^n}(e^{i\tau}) \\ &= \frac{(-i)^{k-1}}{(k-2)!} \frac{(-1)^n}{(n+1)!} \sum_{r=0}^{n+1} \sum_{m=0}^r \binom{n+1}{r} \binom{r}{m} \left(\frac{i}{2}\right)^r (-\pi)^{r-m} \text{LS}_{n+k-(r-m)}^{(k+m-2)}(\tau). \end{aligned} \quad (80)$$

This formula may be used recursively to automatically express the log-sine values $\text{LS}_n^{(k)}(\tau)$ in terms of multiple Clausen and Glaisher functions at τ . Instead of de-

scribing the details, we again only illustrate with a few examples:

$$\text{Ls}_3(\tau) = -2 \text{Gl}_{2,1}(\tau) - \frac{\tau^3}{12} + \frac{\pi\tau^2}{4} - \frac{\pi^2\tau}{4}, \quad (81a)$$

$$\text{Ls}_3^{(1)}(\tau) = \text{Cl}_3(\tau) + \tau \text{Cl}_2(\tau) - \zeta(3), \quad (81b)$$

$$\begin{aligned} \text{Ls}_4(\tau) &= 6 \text{Cl}_{2,1,1}(\tau) - \frac{3}{2} \text{Cl}_4(\tau) - \frac{3(\pi - \tau)}{2} \text{Cl}_3(\tau) \\ &\quad + \frac{3(\pi - \tau)^2}{4} \text{Cl}_2(\tau) + 2\pi\zeta(3), \end{aligned} \quad (81c)$$

$$\text{Ls}_4^{(1)}(\tau) = -2 \text{Gl}_{3,1}(\tau) - 2\tau \text{Gl}_{2,1}(\tau) - \frac{\tau^4}{16} + \frac{\pi\tau^3}{6} - \frac{\pi^2\tau^2}{8} + \frac{\pi^4}{180}, \quad (81d)$$

$$\text{Ls}_4^{(2)}(\tau) = -2 \text{Cl}_4(\tau) + 2\tau \text{Cl}_3(\tau) + \tau^2 \text{Cl}_2(\tau). \quad (81e)$$

Again, as illustrated in Remark 4.2, these evaluations may be obtained using the computer algebra implementations by the authors. For instance, the *Mathematica* code

```
$Assumptions = 0 < t < Pi ;
LsToLi [ Ls [ 4 , 1 , t ] ]
```

produces the evaluation (81d).

In the special case $\tau = \frac{\pi}{3}$ we thus encounter multiple polylogarithms at the basic 6-th root of unity $\omega := \exp(i\pi/3)$. Because their real and imaginary parts satisfy various relations and reductions, studied in [8], the evaluations for log-sine integrals $\text{Ls}_n^{(k)}\left(\frac{\pi}{3}\right)$ can be treated further. For instance, in the cases illustrated for general τ we find the simplified evaluations:

$$\text{Ls}_3\left(\frac{\pi}{3}\right) = -\frac{7\pi^3}{108}, \quad (82a)$$

$$\text{Ls}_3^{(1)}\left(\frac{\pi}{3}\right) = \frac{\pi}{3} \text{Cl}_2\left(\frac{\pi}{3}\right) - \zeta(3), \quad (82b)$$

$$\text{Ls}_4\left(\frac{\pi}{3}\right) = \frac{9}{2} \text{Cl}_4\left(\frac{\pi}{3}\right) + \frac{\pi}{2} \zeta(3), \quad (82c)$$

$$\text{Ls}_4^{(1)}\left(\frac{\pi}{3}\right) = -\frac{17\pi^4}{6480}, \quad (82d)$$

$$\text{Ls}_4^{(2)}\left(\frac{\pi}{3}\right) = -2 \text{Cl}_4\left(\frac{\pi}{3}\right) + \frac{\pi^2}{9} \text{Cl}_2\left(\frac{\pi}{3}\right) + \frac{2\pi}{9} \zeta(3), \quad (82e)$$

$$\text{Ls}_5\left(\frac{\pi}{3}\right) = 6 \text{Gl}_{4,1}\left(\frac{\pi}{3}\right) - \frac{1543}{19440} \pi^5. \quad (82f)$$

Related values at $\pi/3$ can also be found in [19]. The reason that additional relations exist is that the sixth root of unity satisfies the identity $\bar{\omega} = \omega^2$.

The evaluations (73) and (82) together with (71) allow us to give polylogarithmic values for all multiple Mahler measures $\mu_k(1+x+y_*)$. A list of explicit values for the first six cases is given in [12].

Among the polylogarithmic values for $\text{Ls}_n^{(k)}\left(\frac{\pi}{3}\right)$, as illustrated in (82), the first value that is presumed *irreducible* is $\text{Gl}_{4,1}\left(\frac{\pi}{3}\right)$. In general, irreducibility means that a polylogarithmic value is not expressible as a sum of products of lower dimensional polylogarithmic values. Conjectures concerning the number of irreducibles at each depth can be found in [8] in the case of Clausen and Glaisher values, and in [52] for polylogarithms in general. It is worth emphasizing that all such conjectures are necessarily experimental — they would collapse in the unlikely event that it were shown that some odd ζ -value, say $\zeta(11)$, was rational!

Yet, it is possible to express $\text{Gl}_{4,1}\left(\frac{\pi}{3}\right)$ in terms of one-dimensional series as described in [8]:

$$\begin{aligned} \text{Gl}_{4,1}\left(\frac{\pi}{3}\right) &= \sum_{n=1}^{\infty} \frac{\sum_{k=1}^{n-1} \frac{1}{k}}{n^4} \sin\left(\frac{n\pi}{3}\right) \\ &= \frac{3341}{1632960} \pi^5 - \frac{1}{\pi} \zeta(3)^2 - \frac{3}{4\pi} \sum_{j=1}^{\infty} \frac{1}{j^6 \binom{2j}{j}}. \end{aligned} \quad (83)$$

This is a special case of the general fact that log-sine integrals are intimately related to (inverse) central binomial sums. For instance, (83) is a consequence of the formula

$$\sum_{j=1}^{\infty} \frac{1}{j^{n+2} \binom{2j}{j}} = -\frac{(-2)^n}{n!} \text{Ls}_{n+2}^{(1)}\left(\frac{\pi}{3}\right), \quad (84)$$

obtained in [8]. Similarly, alternating binomial sums are related to log-sinh integrals at $2 \log \rho$ where $\rho = \frac{1+\sqrt{5}}{2}$ is the golden mean.

4.1 A physical connection

Even more generally, in their studies of Feynman diagrams [24, 23] Davydychev and Kalmykov obtain results like

$$\sum_{j=1}^{\infty} \frac{u^j}{j^{n+2} \binom{2j}{j}} = -\sum_{m=0}^n \frac{(-2)^m (2l_\theta)^{n-m}}{m!(n-m)!} \text{Ls}_{m+2}^{(1)}(\theta)$$

where $l_\theta = \log(2 \sin \frac{\theta}{2})$ and $u = 4 \sin^2 \frac{\theta}{2}$. Note that $u = 1$ if $\theta = \frac{\pi}{3}$, and $u = -1$ if $\theta = 2i \log \rho$.

Still, this is just the tip of an iceberg explored in [24, 23]. More involved examples include

$$\sum_{j=1}^{\infty} \frac{u^j}{j^{n+2}} \frac{1}{\binom{2j}{j}} S_2(j-1) = -\frac{1}{6} \sum_{m=0}^n \frac{(-2)^m (2l_\theta)^{n-m}}{m!(n-m)!} \text{Ls}_{m+4}^{(3)}(\theta),$$

and

$$\begin{aligned} \sum_{j=1}^{\infty} \frac{u^j}{j} \frac{1}{\binom{2j}{j}} S_1(j-1) S_1(2j-1) &= \tan \frac{\theta}{2} \left\{ 5 \text{Ls}_3(\pi - \theta) - 5 \text{Ls}_3(\pi) - \text{Ls}_3(\theta) \right. \\ &\quad + \frac{1}{2} \text{Ls}_3(2\theta) - 2 \text{Ls}_2(\theta) L_\theta + 2 \text{Ls}_2(\pi - \theta) l_\theta \\ &\quad \left. - 8 \text{Ls}_2(\pi - \theta) L_\theta - 2\theta l_\theta L_\theta + 4\theta L_\theta^2 + \frac{1}{12} \theta^3 \right\}. \end{aligned}$$

Here, $S_a(n) = \sum_{i=1}^n \frac{1}{i^a}$ are the harmonic numbers of order a and $L_\theta = \log(2 \cos \frac{\theta}{2})$.

The reason why physicists care about these types of binomial sums with nested harmonic terms is that they occur naturally in the ε -expansion of hypergeometric functions, while hypergeometric functions come up in the calculation of Feynman diagrams. On the other hand, the ε -expansion of hypergeometric functions is connected with Mahler measure evaluations that were discussed in Section 3. Indeed, in light of (26), we have

$$\sum_{n=0}^{\infty} \mu_n (1+x+y) \frac{\varepsilon^n}{n!} = W_3(\varepsilon) = \frac{\sqrt{3}}{2\pi} 3^{\varepsilon+1} \frac{\Gamma(1 + \frac{\varepsilon}{2})^2}{\Gamma(\varepsilon + 2)} {}_3F_2 \left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4} \right) \quad (85)$$

so that $\mu_n(1+x+y)$ is essentially determined by the terms in the expansion of the hypergeometric ${}_3F_2$ as a series in ε . This is detailed in [4].

The terms of this ε -expansion can be expressed as follows. As in [22, Appendix B], using the duplication formula $(2a)_{2j} = 4^j (a)_j (a+1/2)_j$ as well as the expansion

$$\frac{(m+a\varepsilon)_j}{(m)_j} = \exp \left[- \sum_{k=1}^{\infty} \frac{(-a\varepsilon)^k}{k} [S_k(j+m-1) - S_k(m-1)] \right] \quad (86)$$

allows us to write

$$\begin{aligned}
{}_3F_2\left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4}\right) &= \sum_{j=0}^{\infty} \frac{(1 + \varepsilon/2)_j^3}{4^j (j!)^2 (3/2 + \varepsilon/2)_j} \\
&= \sum_{j=0}^{\infty} \frac{2}{j+1} \frac{1}{\binom{2(j+1)}{j+1}} \left[\frac{(1 + \varepsilon/2)_j}{j!} \right]^4 \left[\frac{(2 + \varepsilon)_{2j}}{(2j+1)!} \right]^{-1} \\
&= \sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} \exp \left[\sum_{k=1}^{\infty} \frac{(-\varepsilon)^k}{k} A_{k,j} \right], \tag{87}
\end{aligned}$$

where

$$A_{k,j} := S_k(2j-1) - 1 - 4 \frac{S_k(j-1)}{2^k} = \sum_{m=2}^{2j-1} \frac{2(-1)^{m+1} - 1}{m^k}. \tag{88}$$

Using (87) as well as Faà di Bruno's formula for the n -th derivative of the composition on two functions, we can now read off the terms of the ε -expansion

$$[\varepsilon^n] {}_3F_2\left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4}\right) = (-1)^n \sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} \sum \prod_{k=1}^n \frac{A_{k,j}^{m_k}}{m_k! k^{m_k}}, \tag{89}$$

where the inner sum is over all non-negative integers m_1, \dots, m_n such that $m_1 + 2m_2 + \dots + nm_n = n$. The evaluation of $\mu_n(1+x+y)$ thus reduces to the evaluation of various multiple inverse binomial sums. Using known results from [23] then produces the evaluations, [4],

$$\mu_1(1+x+y) = \frac{1}{\pi} \text{Ls}_2\left(\frac{\pi}{3}\right), \tag{90}$$

$$\mu_2(1+x+y) = \frac{3}{\pi} \text{Ls}_3\left(\frac{2\pi}{3}\right) + \frac{\pi^2}{4}. \tag{91}$$

We remark that [31, Theorem 11] incorrectly evaluates $\mu_2(1+x+y)$ as $5\pi^2/54$, see [12]. Moreover, supported by the integer relation algorithm PSLQ we have found that the next two instances can also be expressed in terms of log-sine integrals at $\frac{\pi}{3}$ and $\frac{2\pi}{3}$:

$$\mu_3(1+x+y) \stackrel{?[1]}{=} \frac{6}{\pi} \text{Ls}_4\left(\frac{2\pi}{3}\right) - \frac{9}{\pi} \text{Cl}_4\left(\frac{\pi}{3}\right) - \frac{\pi}{4} \text{Cl}_2\left(\frac{\pi}{3}\right) - \frac{13}{2} \zeta(3), \tag{92}$$

$$\begin{aligned}
\mu_4(1+x+y) &\stackrel{?[2]}{=} \frac{12}{\pi} \text{Ls}_5\left(\frac{2\pi}{3}\right) - \frac{49}{3\pi} \text{Ls}_5\left(\frac{\pi}{3}\right) + \frac{81}{\pi} \text{Gl}_{4,1}\left(\frac{2\pi}{3}\right) \\
&+ 3\pi \text{Gl}_{2,1}\left(\frac{2\pi}{3}\right) + \frac{2}{\pi} \zeta(3) \text{Cl}_2\left(\frac{\pi}{3}\right) + \text{Cl}_2\left(\frac{\pi}{3}\right)^2 - \frac{29}{90} \pi^4. \tag{93}
\end{aligned}$$

Based on extended related numerical computations we believe it is not possible to similarly express $\mu_5(1+x+y)$ in terms of log-sine integrals only. An open question is: what is the most appropriate class of terms?

5 Conclusion

The evaluation of log-sine integrals as polylogarithmic values has been implemented by the authors in the computer algebra systems *Mathematica* and SAGE. The packages are freely available for download at:

<http://arminstraub.com/pub/log-sine-integrals>

At this location the interested reader will also find worksheets containing examples. Some details regarding the implementation can be found in [13]. A basic example of its usage is given in Remark 4.2.

Along the way our log-sine and MZV algorithms uncovered several errors (and filled in gaps) in the literature. For instance, the now automatic evaluation

$$\text{Ls}_5^{(2)}(2\pi) = -\frac{13}{45}\pi^5$$

is given incorrectly in [33, (7.144)] as $7\pi^5/30$. More misprints in [33] have been pointed out for instance in [22]. Similarly, as described in Remark 4.2, the recent [20] which contains various formulae for $\text{Ls}_n^{(k)}(2\pi)$ gives incorrect values in several cases.

As the complexity of computer-assisted results increases, automated simplification, validation and correction tools are more and more important in our work and, we believe, throughout mathematics. This is discussed in [9, 10] and is part of our ongoing research program.

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