Arithmetic aspects of random walks and methods in definite integration

An Abstract
Submitted On The First Day Of May, 2012
To The Department Of Mathematics
In Partial Fulfillment Of The Requirements
Of The School Of Science And Engineering
Of Tulane University
For The Degree Of
Doctor Of Philosophy
By

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Abstract

In the first part of this thesis, we revisit a classical problem: how far does a random walk travel in a given number of steps (of length 1, each taken along a uniformly random direction)? We study the moments of the distribution of these distances as well as the corresponding probability distributions. Although such random walks are asymptotically well understood, very few exact formulas had been known; we supplement these with explicit hypergeometric forms and unearth general structures.

Our investigation of the moments naturally leads us to consider (multiple) Mahler measures. For several families of Mahler measures we are able to give evaluations in terms of log-sine integrals. Therefore, and because of the connections of log-sine integrals with number theory and mathematical physics, we study generalized log-sine integrals and show that they evaluate in terms of the well-studied polylogarithms. A computer algebra implementation of our results demonstrates that a large body of results on log-sine integrals scattered over the literature is now computer-amenable.

The second part is concerned with developing specific methods for evaluating several families of definite integrals arising in diverse contexts (such as calculations in quantum field theories). We also review and illustrate Ramanujan's Master Theorem and show that it generalizes to the method of brackets, which has its roots in the negative dimensional integration method utilized by particle physicists. We then apply this technique to multiple integrals recently studied in a physical context.

Complementary to these symbolic methods, we present an exponentially fast algorithm for numerically integrating rational functions over the real line. This algorithm operates on the coefficients of the rational function instead of evaluating it.

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Chapter 1

Introduction and overview

1.1 Overview

All but the first and last chapters of this thesis correspond to a paper that either has already appeared for publication or which has been accepted for publication.

The work presented in Chapters 2–7 originated from revisiting the classical problem of how far a planar random walk travels in a given number of steps. A summary and introduction is given in Section 1.2. We record here an overview of these chapters:

Chapter 2: [BNSW11] *Some arithmetic properties of short random walk integrals*
(with Jonathan M. Borwein, Dirk Nuyens, James Wan)
published in The Ramanujan Journal, Vol. 26, Nr. 1, 2011, p. 109-132

Chapter 3: [BSW11] *Three-step and four-step random walk integrals*
(with Jonathan M. Borwein, James Wan)
to appear in Experimental Mathematics

Chapter 4: [BSWZ11] *Densities of short uniform random walks*
(with Jonathan M. Borwein, James Wan, Wadim Zudilin (appendix by Don Zagier))
to appear in Canadian Journal of Mathematics

Chapter 5: [BS11c] *Special values of generalized log-sine integrals*
(with Jonathan M. Borwein)
published in Proceedings of ISSAC 2011 (36th International Symposium on Symbolic and Algebraic Computation), ACM Press, Jun 2011, p. 43-50
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Chapter 6: [BS11a] *Log-sine evaluations of Mahler measures*
(with Jonathan M. Borwein)
to appear in Journal of the Australian Mathematical Society

Chapter 7: [BBSW12] *Log-sine evaluations of Mahler measures, part II*
(with David Borwein, Jonathan M. Borwein, James Wan)
to appear in Integers (Selfridge memorial volume)

Chapters 8–13 are concerned with developing specific methods for evaluating several families of definite integrals arising in diverse contexts (such as calculations in quantum field theories). An introduction to this second part is given in Section 1.3. Again, we record the relevant chapters:

Chapter 8: [AEG+11] *Ramanujan's Master Theorem*
(with Tewodros Amdeberhan, Ivan Gonzalez, Marshall Harrison, Victor H. Moll)
to appear in The Ramanujan Journal

Chapter 9: [GMS10] *The method of brackets. Part 2: Examples and applications*
(with Ivan Gonzalez, Victor H. Moll)
published in "Gems in Experimental Mathematics", Contemporary Mathematics, Vol. 517, 2010, p. 157-171

Chapter 10: [MMMS10] *A fast numerical algorithm for the integration of rational functions*
(with Dante Manna, Luis Medina, Victor H. Moll)
published in Numerische Mathematik, Vol. 115, Nr. 2, Apr 2010, p. 289-307

Chapter 11: [AMS09] *Closed-form evaluation of integrals appearing in positronium decay*
(with Tewodros Amdeberhan, Victor H. Moll)
published in Journal of Mathematical Physics, Vol. 50, Nr. 10, Oct 2009, 6 p.

Chapter 12: [AEMS10] *Wallis-Ramanujan-Schur-Feynman*
(with Tewodros Amdeberhan, Olivier Espinosa, Victor H. Moll)
published in American Mathematical Monthly, Vol. 117, Nr. 15, Aug 2010, p. 618-632

Chapter 13: [BBS12] *A sinc that sank*
(with David Borwein, Jonathan M. Borwein)
to appear in American Mathematical Monthly, Vol. 119, Nr. 7, Aug-Sep 2012

Finally, this thesis includes Chapters 14, 15 and 16 which discuss work of a more combinatorial type.

In Chapter 14 we study the divisibility properties of the coefficients $c(n,k)$ defined by

$$(1-k^2x)^{-1/k} = \sum_{n\geq 0} c(n,k)x^n$$

which generalize the central binomial coefficients $c(n,2) = \binom{2n}{n}$. In particular, we show that the coefficients are integers.

In Chapter 15 we consider the problem of deciding whether a given rational function has a power series expansion of entirely positive coefficients. By introducing an elementary transformation that preserves such positivity we prove the positivity of

$$\frac{1}{(1-x)(1-y)+(1-y)(1-z)+(1-z)(1-x)},$$

which goes back at least to Gabor Szegö. We then consider applications of this transformation to more general classes of rational functions.

Chapter 16 establishes a q-analog of the classical binomial congruence

$$\binom{ap}{bp} \equiv \binom{a}{b} \mod p^3,$$

where $p > 3$ is a prime. This resolves a problem posed by George Andrews in [And99].

Chapter 14: [SMA09] *The p-adic valuation of k-central binomial coefficients*
(with Tewodros Amdeberhan, Victor H. Moll)
published in Acta Arithmetica, Vol. 140, 2009, p. 31-42

Chapter 15: [Str08] *Positivity of Szego's rational function*
published in Advances in Applied Mathematics, Vol. 41, Issue 2, Aug 2008, p. 255-264

Chapter 16: [Str11] *A q-analog of Ljunggren's binomial congruence*
published in DMTCS Proceedings: 23rd International Conference on Formal Power Series and Algebraic Combinatorics (FPSAC), Jun 2011, p. 897-902

1.2 Arithmetic aspects of random walks

An n-step uniform random walk starts at the origin of the plane 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 [Pea05a]. He posed the problem of determining the distribution of the distance from the origin after a certain number, say n, of steps. Let $W_n(s)$ denote the sth moment of this distance and p_n the corresponding probability density function. Starting with the integral representation

$$W_n(s) = \int_0^1 \cdots \int_0^1 \left| \sum_{k=1}^n e^{2\pi i t_k} \right|^s \mathrm{d}t_1 \cdots \mathrm{d}t_n \tag{1.1}$$

the moments are studied in detail in Chapters 2 and 3. It is shown that the even moments have the interesting combinatorial evaluation

$$W_n(2k) = \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2. \tag{1.2}$$

The consequent recurrences satisfied by the even moments are lifted to functional equations satisfied by $W_n(s)$. In the cases $n = 3$ and $n = 4$ a more explicit study shows that $W_n(s)$ has a representation as a Meijer G-function. Ultimately, using transformations of Meijer G-functions and identities from the theory of elliptic integrals, this allows us to find closed formulas for the average distances $W_3(1)$ and $W_4(1)$ (in the latter case, as a sum of ${}_6F_5$'s). Previously, only the trivial evaluation $W_2(1) = \frac{4}{\pi}$ was known.

Knowledge of the pole structure of the $W_n(s)$ and the general theory of the (distributional) Mellin calculus allow us to prove in Chapter 4 that the densities p_n satisfy Fuchsian differential equations. Using a family of combinatorial identities discovered in [DM04] (Don Zagier kindly provided his direct combinatorial proof as an appendix to Chapter 4) we show that the singularities of p_n occur at the positive integers

$n, n-2, \ldots$ as well as 0. Surprisingly, we find that in the cases $n = 3$ and $n = 4$ the differential equations arise from modular forms (more precisely, in each case there is a modular form $f(\tau)$ and a modular function $g(\tau)$ such that the function y locally expressing $f(\tau) = y(g(\tau))$ satisfies the differential equation at hand). Moreover, we are able to give the hypergeometric evaluation

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16 - x^2}}{x} \operatorname{Re} {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \middle| \frac{(16 - x^2)^3}{108 x^4} \right) \tag{1.3}$$

valid throughout $0 \leqslant x \leqslant 4$; this complements the classically known expressions for p_2 and p_3. Further exploiting the mentioned modularity of p_4 and the Chowla-Selberg formula we find that $p_4(1)$ is expressible as $\frac{\sqrt{5}}{40\pi^4} \Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})$. From general principles this gives the first residue of W_5 and thus the first term in the expansion of p_5 for small argument. Based on numerical experiments, we conjecture a related expression for the second residue. Combined, this characterizes p_5 for small argument as a particular solution to a Calabi-Yau type differential equation [AvEvSZ10].

The *multiple Mahler measure*, recently introduced in [KLO08], of k functions $P_1, \ldots, P_k$ (typically Laurent polynomials) in n variables is defined as

$$\mu(P_1, P_2, \ldots, P_k) = \int_0^1 \cdots \int_0^1 \prod_{j=1}^{k} \log \left| P_j \left(e^{2\pi i t_1}, \ldots, e^{2\pi i t_n} \right) \right| \mathrm{d}t_1 \mathrm{d}t_2 \ldots \mathrm{d}t_n. \tag{1.4}$$

When $k = 1$ this reduces to the standard (logarithmic) *Mahler measure* [Boy98]. The moments of random walks W_n are related to Mahler measures: the derivatives $W_n^{(k)}(0)$ equal the multiple Mahler measure $\mu_k(1+x_1+\ldots+x_{n-1})$ where $\mu_k(P) = \mu(P_1, \ldots, P_k)$ with $P_1, \ldots, P_k = P$.

A Mahler measure of similar form was studied by Sasaki [Sas10] who considered $\mu(1+x+y_1, 1+x+y_2, \ldots, 1+x+y_k)$ and provided an evaluation of $\mu(1+x+y_1, 1+x+y_2)$. We show in Chapter 6 that this Mahler measure has a natural evaluation in terms of *log-sine integrals*. Namely, if

$$\mathrm{Ls}_n^{(k)}(\sigma) = -\int_0^\sigma \theta^k \log^{n-1-k}\left|2\sin\frac{\theta}{2}\right| \mathrm{d}\theta \tag{1.5}$$

denotes the (generalized) log-sine integral then

$$\mu(1+x+y_1,\ldots,1+x+y_k) = \frac{1}{\pi}\mathrm{Ls}_{k+1}\left(\frac{\pi}{3}\right) - \frac{1}{\pi}\mathrm{Ls}_{k+1}(\pi)\,. \tag{1.6}$$

In Chapters 6 and 7 we demonstrate that several other Mahler measures have values involving generalized log-sine integrals at π, $\pi/3$ or more general arguments. Accordingly, we analyze in Chapter 5 log-sine integrals and their evaluations, both explicit and in terms of generating series. We show that log-sine integrals can be systematically evaluated in terms of polylogarithms of Nielsen type at corresponding argument. This approach unifies (and automatizes) various results found in the literature (and rectifies several errors; see Chapter 5 and [BS11b]). The implementation of our results in the computer algebra systems *SAGE* and *Mathematica* complements existing computer algebra packages such as `lsjk` [KS05] for numerical evaluations of log-sine integrals, or `HPL` [Mai06] as well as [VW05] for working with multiple polylogarithms. These packages are used, for instance, in particle physics [DK00, KV00] where log-sine integrals appeared in recent work on the higher-order terms in the ε-expansion of various Feynman diagrams.

1.3 Methods in definite integration

Many families of definite integrals can be evaluated using *Ramanujan's Master Theorem* (RMT, henceforth)

$$\int_0^\infty x^{s-1} \left\{ \lambda(0) - \frac{x}{1!}\lambda(1) + \frac{x^2}{2!}\lambda(2) - \cdots \right\} \mathrm{d}x = \Gamma(s)\lambda(-s). \tag{1.7}$$

As an application we show in Chapter 8 that David Broadhurst's Bessel integral representation [Bro09] of the moments $W_n(s)$ of random walks can be derived naturally:

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x} \right)^k J_0^n(x)\, \mathrm{d}x \tag{1.8}$$

for $2k > \operatorname{Re} s > \max(-2, -\frac{n}{2})$. Moreover, we demonstrate that RMT can be used to explain the *method of brackets*, a method for evaluating multidimensional definite integrals first presented in [GS07] in the context of integrals arising from Feynman diagrams. While the basic idea is the assignment of a formal symbol $\langle a \rangle$ to the divergent integral

$$\int_0^\infty x^{a-1}\, \mathrm{d}x, \tag{1.9}$$

we refer to [GM10] or Chapter 9 for a complete description of the operational rules. The method is similar, as discussed in Section 17.1.2, to the approach of repeatedly introducing Mellin-Barnes integral representations inside an integral but has purely algebraic rules. This makes the method particularly interesting for implementation in a computer algebra system, a project initiated by Karen Kohl [Koh11] in her thesis. The price to pay for not having to care about the contours of integration in the complex plane and keeping track of the appropriate set of residues is that the method of brackets, in its current formulation, is heuristic in the sense that an evaluation does not constitute rigorous proof, see Section 17.1.2. We demonstrate the utility of the method in Chapter 9 by applying it to several integrals of physical interest including the loop integral (in Schwinger parametrization), also considered in [BD91], associated to a single-loop Feynman diagram (with one independent external momentum and one massive denominator)

$$\int_0^\infty \int_0^\infty \int_0^\infty x_1^{a_1-1} x_2^{a_2-1} x_3^{a_3-1} \frac{\exp\left(x_1 m^2\right) \exp\left(-\frac{x_1 x_2}{x_1+x_2+x_3} s\right)}{\left(x_1+x_2+x_3\right)^{D/2}} \, \mathrm{d}x_1 \, \mathrm{d}x_2 \, \mathrm{d}x_3 \tag{1.10}$$

which is evaluated in terms of hypergeometric functions in each of the regions $|s/m^2| < 1$ and $|s/m^2| > 1$. An advantage of the method of brackets is that it obtains both results without the need for analytic continuation.

By using the theory of rational Landen transformations (which mimics the classical elliptic Landen transformation [MM08a]), we devise an exponentially fast algorithm in Chapter 10 for numerically integrating rational functions over the real line to high precision. The algorithm defines a dynamical system on the coefficients of the rational integrand which at each step preserves the integral on the line. The transformations are given by explicit polynomials which depend on the degree of the input and the desired order of the method (both of which are arbitrary). We analyze the complexity of the algorithm and provide an implementation for *Mathematica*.

In Chapters 11, 12 and 13 we study specific families of definite integrals which are briefly indicated next. In Chapter 11 we give an analytic evaluation involving the dilogarithm function for two integrals including

$$\int_0^1 \frac{\log[x_1 + (1-x_1)y^2]}{(1-x_1)x_2 - x_1(1-x_2)y^2} \, \mathrm{d}y \tag{1.11}$$

which were recently studied in the context of quantum field theories. In Chapter 12 we generalize a classical integral evaluation of Wallis to the integral

$$\int_0^\infty \prod_{k=1}^n \frac{1}{x^2 + q_k^2} \, \mathrm{d}x \tag{1.12}$$

which is evaluated as a quotient of Schur functions. Various applications are given, including to a sum related to Feynman diagrams. Lastly, in Chapter 13 we consider and evaluate the sinc integral

$$\int_{-\infty}^{\infty} \prod_{j=1}^{n} \frac{\sin\left(k_j(x-a_j)\right)}{x-a_j}\,\mathrm{d}x \tag{1.13}$$

which had been posed as a MONTHLY problem but whose solution was subsequently withdrawn.

1.4 Some notation

We collect here some notation which is common to Chapters 5, 6, 7 and thus reproduced here.

The *multiple polylogarithm*, as studied for instance in [BBK01] and [BBG04, Ch. 3], will be denoted by

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

For our purposes, the $a_1,\ldots,a_k$ will usually be positive integers and $a_1 \geqslant 2$ so that the sum converges for all $|z| \leqslant 1$. For example, $\mathrm{Li}_{2,1}(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2} \sum_{j=1}^{k-1} \frac{1}{j}$. In particular, $\mathrm{Li}_k(x) := \sum_{n=1}^{\infty} \frac{x^n}{n^k}$ is the *polylogarithm of order* k and

$$\mathrm{Ti}_k(x) := \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)^k}$$

the related *inverse tangent of order* k. We use the same notation for the analytic continuations of these functions. The usual notation will be used for repetitions so that, for instance, $\mathrm{Li}_{2,\{1\}^3}(z) = \mathrm{Li}_{2,1,1,1}(z)$.

Moreover, *multiple zeta values* are denoted by

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

Similarly, we consider the *multiple Clausen functions* (Cl) and *multiple Glaisher functions* (Gl) of depth k and weight $w = a_1 + \ldots + a_k$ defined as

$$\mathrm{Cl}_{a_1,\ldots,a_k}(\theta) = \left\{ \begin{array}{ll} \mathrm{Im}\ \mathrm{Li}_{a_1,\ldots,a_k}(e^{i\theta}) & \text{if } w \text{ even} \\ \mathrm{Re}\ \mathrm{Li}_{a_1,\ldots,a_k}(e^{i\theta}) & \text{if } w \text{ odd} \end{array} \right\}, \tag{1.14}$$

$$\mathrm{Gl}_{a_1,\ldots,a_k}(\theta) = \left\{ \begin{array}{ll} \mathrm{Re}\ \mathrm{Li}_{a_1,\ldots,a_k}(e^{i\theta}) & \text{if } w \text{ even} \\ \mathrm{Im}\ \mathrm{Li}_{a_1,\ldots,a_k}(e^{i\theta}) & \text{if } w \text{ odd} \end{array} \right\}, \tag{1.15}$$

in accordance with [Lew81]. Thus

$$\mathrm{Ls}_2(\theta) = \mathrm{Cl}_2(\theta) = \sum_{n=1}^{\infty} \frac{\sin(n\theta)}{n^2}. \tag{1.16}$$

As illustrated by (1.16) and later in (5.28), the Clausen and Glaisher functions alternate between being cosine and sine series with the parity of the dimension. Of particular importance will be the case of $\theta = \pi/3$ which has also been considered in [BBK01].

Finally, we recall the following Kummer-type polylogarithm, [Lew81, BBK01], which has been exploited in [BZB08] among other places:

$$\lambda_n(x) := (n-2)! \sum_{k=0}^{n-2} \frac{(-1)^k}{k!} \mathrm{Li}_{n-k}(x) \log^k |x| + \frac{(-1)^n}{n} \log^n |x|, \tag{1.17}$$

so that

$$\lambda_1\left(\tfrac{1}{2}\right) = \log 2, \quad \lambda_2\left(\tfrac{1}{2}\right) = \frac{1}{2}\zeta(2), \quad \lambda_3\left(\tfrac{1}{2}\right) = \frac{7}{8}\zeta(3),$$

and $\lambda_4\left(\frac{1}{2}\right)$ is the first to reveal the presence of $\mathrm{Li}_n\left(\frac{1}{2}\right)$.

Our other notation and usage in Chapters 5, 6, 7 is largely consistent with that in [Lew81] and that in the newly published [OLBC10] 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 [BC10].

Chapter 2

Some arithmetic properties of short random walk integrals

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[BNSW11] *Some arithmetic properties of short random walk integrals*
(with Jonathan M. Borwein, Dirk Nuyens, James Wan)
published in The Ramanujan Journal, Vol. 26, Nr. 1, 2011, p. 109-132

Abstract We study the moments of the distance traveled by a walk in the plane with unit steps in random directions. While this historically interesting random walk is well understood from a modern probabilistic point of view, our own interest is in determining explicit closed forms for the moment functions and their arithmetic values at integers when only a small number of steps is taken. As a consequence of a more general evaluation, a closed form is obtained for the average distance traveled in three steps. This evaluation, as well as its proof, rely on explicit combinatorial properties, such as recurrence equations of the even moments (which are lifted to functional equations). The corresponding general combinatorial and analytic features are collected and made explicit in the case of 3 and 4 steps. Explicit hypergeometric expressions are given for the moments of a 3-step and 4-step walk and a general conjecture for even length walks is made.

2.1 Introduction, history and preliminaries

We consider, for various values of s, the n-dimensional integral

$$W_n(s) := \int_{[0,1]^n} \left| \sum_{k=1}^{n} e^{2\pi i x_k} \right|^s \mathrm{d}\boldsymbol{x} \tag{2.1}$$

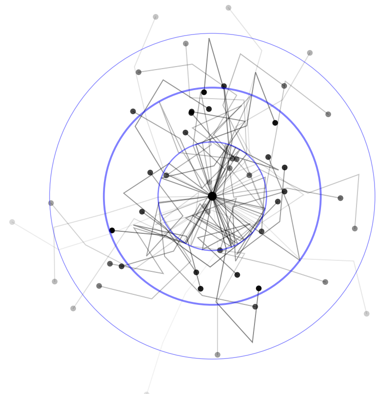
which occurs in the theory of uniform random walks in the plane, where at each step a unit-step is taken in a random direction, see Figure 2.1. As such, the integral (2.1) expresses the s-th moment of the distance to the origin after n steps. Our interest in these integrals is from the point of view of (symbolic) computation. In particular, we seek explicit closed forms of the moment functions $W_n(s)$ for small n as well as closed form evaluations of these functions at integer arguments. Of special interest is the case $W_n(1)$ of the expected distance after n steps.

While the general structure of the moments and densities of the random walks studied here is well-known from a modern probabilistic point of view (for instance, the characteristic function of the distance after n steps is simply the Bessel function J_0^n—a fact reflected in (2.14) and (2.28)), there has been little research on the question of closed forms. This is exemplified by the fact that $W_3(1)$ has apparently not been evaluated in the literature before (in contrast the case $W_2(1) = \frac{4}{\pi}$ is easy). As a consequence of a more general result we show in Section 2.5 that

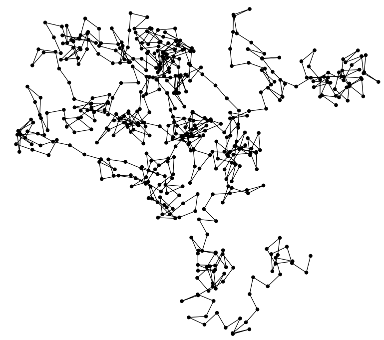
$$W_3(1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4} \frac{2^{2/3}}{\pi^4} \Gamma^6\left(\frac{2}{3}\right) \tag{2.2}$$

where Γ is the *gamma function*.

A related second motivation for our work is of a numerical nature. In fact, more than 70 years after the problem was posed, [MFW77] remarks that for the densities of 4, 5 and 6-steps walks, "it has remained difficult to obtain reliable values". One challenge lies in the difficulty of computing the involved integrals, such as (2.28)



(a) Several 4-step walks



(b) A 500-step walk

Figure 2.1: Random walks in the plane.

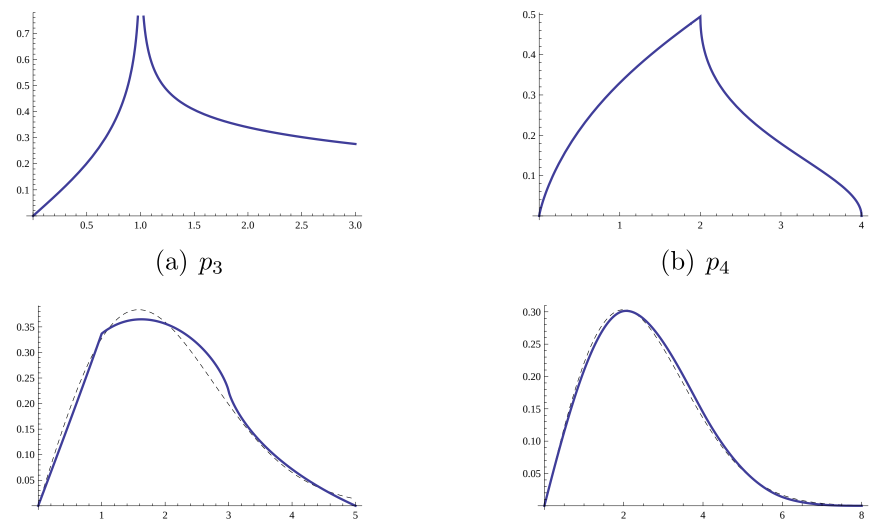
which is highly oscillatory, to reasonably high precision. This is not straightforward, and so some comments on obtaining high precision numerical evaluations of $W_n(s)$ are given in Appendix 2.6.2. A more comprehensive study of the numerics of such multiple-integrations is conducted in [BB11].

The term "random walk" first appears in a question by Karl Pearson in *Nature* in 1905 [Pea05a]. He asked for the probability density of a two-dimensional random walk couched in the language of how far a "rambler" (hill walker) might walk. This triggered a response by Lord Rayleigh [Ray05] 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 probability distribution $\frac{2x}{n}e^{-x^2/n}$ for large n. This quickly leads to a good approximation for $W_n(s)$ for large n and fixed $s = 1, 2, 3, \ldots$.

Another week later, Pearson again wrote in *Nature*, see [Pea05b], 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 *complete elliptic integral* of the first kind K. This density function can be written as

$$p_3(x) = \operatorname{Re}\left(\frac{\sqrt{x}}{\pi^2}\,K\left(\sqrt{\frac{(x+1)^3(3-x)}{16x}}\right)\right), \tag{2.3}$$

see, e.g., [Hug95] and [Pea06]. Pearson 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 2.2: while p_8 is visually almost indistinguishable from the smooth limiting form (shown in superimposed dotted lines) given by Rayleigh, the densities p_3, p_4 and p_5 have remarkable features of their own.



(a) p_3

(b) p_4

(c) p_5

(d) p_8

Figure 2.2: Densities p_3, p_4, p_5 and, for contrast, p_8.

The results obtained here, as well as in a follow-up study in [BSW11], have been crucial in the discovery ([BSWZ11]) of a closed form for the density p_4 of the distance traveled in 4 steps. Additionally, an improved hypergeometric evaluation of p_3 is obtained in [BSWZ11]. For the convenience of the reader, the closed forms obtained in [BSWZ11] are:

$$p_3(x) = \frac{2\sqrt{3}}{\pi} \frac{x}{(3+x^2)} {}_2F_1\left(\left. \begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \right| \frac{x^2\left(9-x^2\right)^2}{\left(3+x^2\right)^3} \right), \tag{2.4}$$

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16-x^2}}{x} \operatorname{Re} {}_3F_2\left(\left. \begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \right| \frac{\left(16-x^2\right)^3}{108x^4} \right), \tag{2.5}$$

for $0 \leqslant x \leqslant 3$ and $0 \leqslant x \leqslant 4$ respectively.

It should be noted that the progress we make here (and in [BSW11, BSWZ11]) on the question of closed forms rely on techniques, for instance analysis of Meijer G-functions and their relationship with generalized hypergeometric series, that were fully developed only much later in the 20th century.

We remark that much has been done in generalizing the problem posed by Pearson. For instance, in further response to Pearson, Kluyver [Klu06] made a lovely analysis of the cumulative distribution function of the distance traveled by a rambler in the plane for various choices of step length. Other generalizations include allowing walks in three dimensions (where the analysis is actually simpler, see [Wat41, §49]), confining the walks to different kinds of lattices, or calculating whether and when the walker would return to the origin. An excellent source of this sort of results is [Hug95].

Applications of two-dimensional random walks are numerous and well-known; for instance, [Hug95] mentions that they may be used to model the random migration of an organism possessing flagella; analysing the superposition of waves (e.g., from a laser beam bouncing off an irregular surface); and vibrations of arbitrary frequencies. The subject also finds use in Brownian motion and quantum chemistry.

We learned of the special case for $s = 1$ of (2.1) from the whiteboard in the common room at the University of New South Wales. It had been written down by Peter Donovan as a generalization of a discrete cryptographic problem, as discussed in [Don09]. Some numerical values of W_n evaluated at integers are shown in Tables 2.1 and 2.2. One immediately notices the apparent integrality of the sequences for the even moments—which are the moments of the squared expected distance, and where the square root for $s = 2$ gives the root-mean-square distance $\sqrt{n}$. For $n = 2, 3, 4$ these sequences were found in the Online Encyclopedia of Integer Sequences [Slo09]—the cases $n = 5, 6$ are in the database as a consequence of this paper.

n	$s=2$	$s=4$	$s=6$	$s=8$	$s=10$	[Slo09]
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 2.1: $W_n(s)$ at even integers.

n	$s=1$	$s=3$	$s=5$	$s=7$	$s=9$
2	1.27324	3.39531	10.8650	37.2514	132.449
3	1.57460	6.45168	36.7052	241.544	1714.62
4	1.79909	10.1207	82.6515	822.273	9169.62
5	2.00816	14.2896	152.316	2037.14	31393.1
6	2.19386	18.9133	248.759	4186.19	82718.9

Table 2.2: $W_n(s)$ at odd integers.

By numerical observation, experimentation and some sketchy arguments we quickly conjectured and strongly believed that, for k a nonnegative integer

$$W_3(k) = \mathrm{Re}\ {}_3F_2\left(\left.\begin{matrix}\frac{1}{2}, -\frac{k}{2}, -\frac{k}{2} \\ 1, 1\end{matrix}\right| 4\right). \tag{2.6}$$

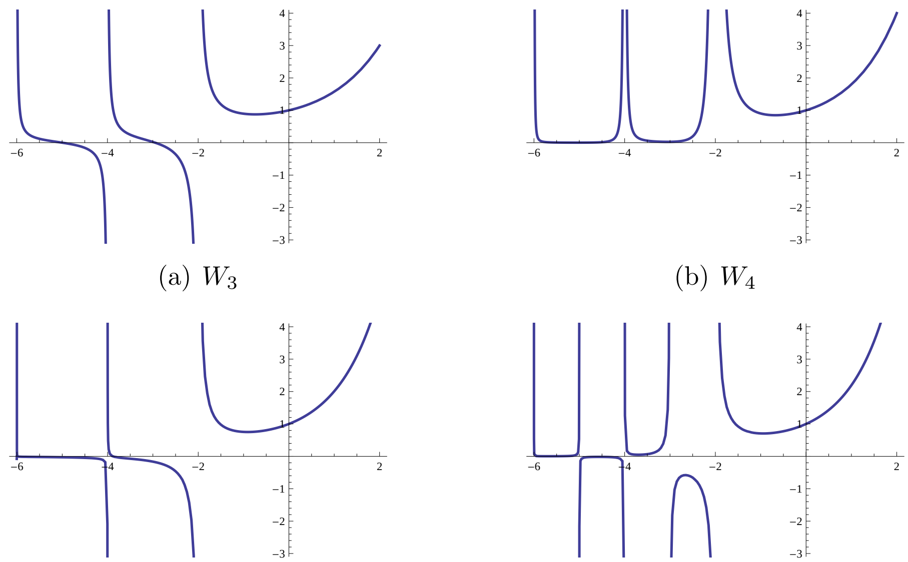
The evaluation (2.2) of $W_3(1)$ can be deduced from (2.6). Based on results in Sections 2.2 and 2.3, the evaluation (2.6) is established in Section 2.5.

In Section 2.2 we observe that the even moments $W_n(2k)$ are given by integer sequences and study the combinatorial features of $f_n(k) := W_n(2k)$, k a nonnegative integer. We show that there is a recurrence relation for the numbers $f_n(k)$ and confirm an observation from Table 2.1 that the last digit in the column for $s = 10$ is always n mod 10. The discovery of (2.6) was precipitated by the form of f_3 given in (2.12).

In Section 2.3 some analytic results are collected, and the recursions for $f_n(k)$ are lifted to $W_n(s)$ by the use of Carlson's theorem. The recursions for $n = 2, 3, 4, 5$ are given explicitly as an example. These recursions then give further information regarding the pole structure of $W_n(s)$. Plots of the analytic continuation of $W_n(s)$ on the negative real axis are given in Figure 2.3. Inspired by a more general combinatorial convolution given in Section 2.2 we conjecture, for $n = 1, 2, \ldots$, the recursion

$$W_{2n}(s) \stackrel{?}{=} \sum_{j \geqslant 0} \binom{s/2}{j}^2 W_{2n-1}(s-2j),$$

which has been partially resolved in [BSW11].



(a) W_3 (b) W_4 (c) W_5 (d) W_6

Figure 2.3: Various W_n and their analytic continuations.

2.2 The even moments and their combinatorial features

In the case $s = 2k$ the square root implicit in the definition (2.1) of $W_n(s)$ disappears, resulting in the fact that the even moments $W_n(2k)$ are integers. In this section we collect several of the combinatorial features of these moments which, while sometimes in principle routine, provide important guidance and foundation. For instance, the combinatorial expression for $W_3(2k)$ will eventually lead to the evaluation of all integer moments $W_3(k)$ in Section 2.5. As a second example, the recurrence equation, in its explicit form, for $W_4(2k)$ is at the heart of the derivation of the closed form (2.5) in [BSWZ11].

In fact, the even moments are given as sums of squares of multinomials—as is detailed next. While this result may be readily obtained from general probabilistic principles starting with the observation that the characteristic function of the distance traveled in n steps is given by the Bessel function J_0^n (see Section 2.4), we prefer to give an elementary derivation starting from the integral definition (2.1) of $W_n(s)$.

Proposition 2.2.1. *For nonnegative integers k and n,*

$$W_n(2k) = \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1,\ldots,a_n}^2.$$

Proof. In the spirit of the residue theorem of complex analysis, if $f(x_1,\ldots,x_n)$ has a Laurent expansion around the origin then

$$\operatorname{ct} f(x_1,\ldots,x_n) = \int_{[0,1]^n} f(e^{2\pi \mathrm{i} x_1},\ldots,e^{2\pi \mathrm{i} x_n})\,\mathrm{d}\boldsymbol{x}, \tag{2.7}$$

where 'ct' denotes the operator which extracts from an expression the constant term of its Laurent expansion. In light of (2.7), the integral definition (2.1) of $W_n(s)$ may be restated as

$$W_n(s) = \operatorname{ct}\left((x_1+\cdots+x_n)(1/x_1+\cdots+1/x_n)\right)^{s/2}, \tag{2.8}$$

see also Appendix 2.6.1. In the case $s = 2k$ the right-hand side may be finitely expanded to yield the claim: on using the multinomial theorem,

$$\begin{aligned}(x_1+&\cdots+x_n)^k\,(1/x_1+\cdots+1/x_n)^k \\ &= \sum_{a_1+\cdots+a_n=k}\binom{k}{a_1,\ldots,a_n} x_1^{a_1}\cdots x_n^{a_n} \sum_{b_1+\cdots+b_n=k}\binom{k}{b_1,\ldots,b_n} x_1^{-b_1}\cdots x_n^{-b_n},\end{aligned}$$

and the constant term is now obtained by matching $a_1 = b_1, \ldots, a_n = b_n$. $\square$

Remark 2.2.2. In the case that s is not an even integer, the right-hand side of (2.8) may still be expanded, say, when Re $s \geqslant 0$ to obtain the series evaluation

$$W_n(s) = n^s \sum_{m \geqslant 0} (-1)^m \binom{s/2}{m} \sum_{k=0}^{m} \frac{(-1)^k}{n^{2k}} \binom{m}{k} \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2. \tag{2.9}$$

An alternative elementary proof of this expansion is given in Appendix 2.6.1. We include this alternative proof, which chronologically was our first one, because, as a side-product, it yields other interesting integral evaluations. $\diamondsuit$

In light of Proposition 2.2.1, we consider the combinatorial sums

$$f_n(k) = \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2. \tag{2.10}$$

of multinomial coefficients squared. These numbers also appear in [RS09] in the following way: $f_n(k)$ counts the number of *abelian squares* of length $2k$ over an alphabet with n letters (that is strings xx' of length $2k$ from an alphabet with n letters such that x' is a permutation of x). It is not hard to see that

$$f_{n_1+n_2}(k) = \sum_{j=0}^{k} \binom{k}{j}^2 f_{n_1}(j)\, f_{n_2}(k-j), \tag{2.11}$$

for two non-overlapping alphabets with n_1 and n_2 letters. In particular, we may use (2.11) to obtain $f_1(k) = 1$, $f_2(k) = \binom{2k}{k}$, as well as

$$f_3(k) = \sum_{j=0}^{k} \binom{k}{j}^2 \binom{2j}{j} = {}_3F_2\left(\left.\begin{matrix}\frac{1}{2}, -k, -k \\ 1, 1\end{matrix}\right| 4\right) = \binom{2k}{k} {}_3F_2\left(\left.\begin{matrix}-k, -k, -k \\ 1, -k+\frac{1}{2}\end{matrix}\right| \frac{1}{4}\right), \tag{2.12}$$

$$f_4(k) = \sum_{j=0}^{k} \binom{k}{j}^2 \binom{2j}{j} \binom{2(k-j)}{k-j} = \binom{2k}{k} {}_4F_3\left(\left.\begin{matrix}\frac{1}{2}, -k, -k, -k \\ 1, 1, -k+\frac{1}{2}\end{matrix}\right| 1\right). \tag{2.13}$$

Here and below ${}_pF_q$ notates the generalised hypergeometric function. In general, (2.11) can be used to write f_n as a sum with at most $\lceil n/2 \rceil - 1$ summation indices.

We recall a generating function for $(f_n(k))_{k=0}^{\infty}$ used in [BBBG08]. Let $I_n(z)$ denote the *modified Bessel function* of the first kind. Then

$$\sum_{k \geqslant 0} f_n(k) \frac{z^k}{(k!)^2} = \left(\sum_{k \geqslant 0} \frac{z^k}{(k!)^2} \right)^n = {}_0F_1(1; z)^n = I_0(2\sqrt{z})^n. \tag{2.14}$$

It can be anticipated from (2.10) that, for fixed n, the sequence $f_n(k)$ will satisfy a linear recurrence with polynomial coefficients. A procedure for constructing these recurrences has been given in [Bar64]; in particular, that paper gives the recursions for $3 \leqslant n \leqslant 6$ explicitly. Moreover, an explicit general formula for the recurrences is given in [Ver04]:

Theorem 2.2.3. *For fixed $n \geqslant 2$, the sequence $f_n(k)$ satisfies a recurrence of order $\lambda = \lceil n/2 \rceil$ with polynomial coefficients of degree $n-1$:*

$$\sum_{j \geqslant 0} \left[k^{n-1} \sum_{\alpha_1, \ldots, \alpha_j} \prod_{i=1}^{j} -\alpha_i(n+1-\alpha_i) \left(\frac{k-i}{k-i+1} \right)^{\alpha_i - 1} \right] f_n(k-j) = 0. \tag{2.15}$$

Here, the sum is over all sequences $\alpha_1, \ldots, \alpha_j$ such that $0 \leqslant \alpha_i \leqslant n$ and $\alpha_{i+1} \leqslant \alpha_i - 2$.

The recursions for $n = 2, 3, 4, 5$ are listed in Example 2.3.4 in Section 2.3.3, formulated in terms of $W_n(s)$ as per Theorem 2.3.3. As a consequence of Theorem 2.2.3 we obtain:

Theorem 2.2.4. *For fixed $n \geqslant 2$, the sequence $f_n(k)$ satisfies a recurrence of order $\lambda = \lceil n/2 \rceil$ with polynomial coefficients of degree $n-1$:*

$$c_{n,0}(k) f_n(k) + \cdots + c_{n,\lambda}(k) f_n(k+\lambda) = 0 \tag{2.16}$$

where

$$c_{n,0}(k) = (-1)^{\lambda} (n!!)^2 \left(k + \frac{n}{4}\right)^{n+1-2\lambda} \prod_{j=1}^{\lambda-1} (k+j)^2 , \tag{2.17}$$

and $c_{n,\lambda}(k) = (k+\lambda)^{n-1}$. *Here* $n!! = \prod_{i=0}^{\lambda-1}(n-2i)$ *is the double factorial.*

Proof. The claim for $c_{n,\lambda}$ follows straight from (2.15). By (2.15), $c_{n,0}$ is given by

$$c_{n,0}(k-\lambda) = \left[k^{n-1} \sum_{\alpha_1,\ldots,\alpha_\lambda} \prod_{i=1}^{\lambda} -\alpha_i(n+1-\alpha_i) \left(\frac{k-i}{k-i+1}\right)^{\alpha_i-1} \right] \tag{2.18}$$

where the sum is again over all sequences $\alpha_1, \ldots, \alpha_\lambda$ such that $0 \leqslant \alpha_i \leqslant n$ and $\alpha_{i+1} \leqslant \alpha_i - 2$.

If n is odd then there is only one such sequence, namely $\{n, n-2, n-4, \ldots\}$, and it follows that

$$c_{n,0}(k-\lambda) = (-1)^{\lambda} (n!!)^2 \prod_{j=1}^{\lambda-1} (k-j)^2 \tag{2.19}$$

in accordance with (2.17).

When $n = 2\lambda$ is even, there are $\lambda+1$ sequences, namely $\alpha^0 = \{n, n-2, n-4, \ldots, 2\}$, and α^i for $1 \leqslant i \leqslant \lambda$, where α^i is constructed from α^0 by subtracting all elements by 1 starting from the $(\lambda+1-i)$th position.

Now by (2.18), we have

$$c_{n,0}(k-\lambda) = (-1)^{\lambda} \left(\prod_{i=1}^{\lambda-1}(k-i)^2\right) \sum_{j=0}^{\lambda} \left(\prod_{i=1}^{\lambda} a_i^j(n+1-a_i^j)\right)(k-\lambda+j), \tag{2.20}$$

where a_i^j denotes the ith element of a^j.

We make the key observation that the sum in (2.20) is symmetric, so writing it backwards and adding that to itself, we factor out the term involving k:

$$2\sum_{j=0}^{\lambda} \left(\prod_{i=1}^{\lambda} a_i^j(n+1-a_i^j)\right)(k-\lambda+j) = (2k-\lambda)\sum_{j=0}^{\lambda}\prod_{i=1}^{\lambda} a_i^j(n+1-a_i^j). \tag{2.21}$$

As we know the sequences a^j explicitly, the product on the right of (2.21) simplifies to

$$(2\lambda)!\frac{\binom{2j}{j}\binom{2\lambda-2j}{\lambda-j}}{\binom{2\lambda}{\lambda}}.$$

Hence the sum on the right of (2.21) is

$$\sum_{j=0}^{\lambda}(2\lambda)!\frac{\binom{2j}{j}\binom{2\lambda-2j}{\lambda-j}}{\binom{2\lambda}{\lambda}} = 2^{2\lambda}\lambda!^2, \tag{2.22}$$

which can be verified, for instance, using the snake oil method ([Wil90]). Substituting this into (2.20) gives (2.17) for even n. □

Remark 2.2.5. For fixed k, the map $n \mapsto f_n(k)$ can be given by the evaluation of a polynomial in n of degree k. This follows from

$$f_n(k) = \sum_{j=0}^{k}\binom{n}{j}\sum_{\substack{a_1+\cdots+a_j=k \\ a_i>0}}\binom{k}{a_1,\ldots,a_j}^2, \tag{2.23}$$

because the right-hand side is a linear combination (with positive coefficients only depending on k) of the polynomials $\binom{n}{j} = \frac{n(n-1)\cdots(n-j+1)}{j!}$ in n of degree j for $j = 0, 1, \ldots, k$.

From (2.23) the coefficient of $\binom{n}{k}$ is seen to be $(k!)^2$. We therefore formally obtain the first-order approximation $W_n(s) \approx_n n^{s/2}\Gamma(s/2+1)$ for n going to infinity, see also [Klu06]. In particular, $W_n(1) \approx_n \sqrt{n\pi}/2$. Similarly, the coefficient of $\binom{n}{k-1}$ is $\frac{k-1}{4}(k!)^2$ which gives rise to the second-order approximation

$$(k!)^2\binom{n}{k} + \frac{k-1}{4}(k!)^2\binom{n}{k-1} = k!n^k - \frac{k(k-1)}{4}\,k!n^{k-1} + O(n^{k-2})$$

of $f_n(k)$. We therefore obtain

$$W_n(s) \approx_n n^{s/2-1}\left\{\left(n-\frac{1}{2}\right)\Gamma\left(\frac{s}{2}+1\right) + \Gamma\left(\frac{s}{2}+2\right) - \frac{1}{4}\Gamma\left(\frac{s}{2}+3\right)\right\},$$

which is exact for $s = 0, 2, 4$. In particular, $W_n(1) \approx_n \sqrt{n\pi}/2 + \sqrt{\pi/n}/32$. More general approximations are given in [Cra09]. $\diamondsuit$

Remark 2.2.6. It follows straight from (2.10) that, for primes p, $f_n(p) \equiv n$ modulo p. Further, for $k \geqslant 1$, $f_n(k) \equiv n$ modulo 2. This may be derived inductively from the recurrence (2.11) since, assuming that $f_n(k) \equiv n$ modulo 2 for some n and all $k \geqslant 1$,

$$f_{n+1}(k) = \sum_{j=0}^{k} \binom{k}{j}^2 f_n(j) \equiv 1 + \sum_{j=1}^{k} \binom{k}{j} n = 1 + n(2^k - 1) \equiv n + 1 \pmod 2.$$

Hence for odd primes p,

$$f_n(p) \equiv n \pmod{2p}. \tag{2.24}$$

The congruence (2.24) also holds for $p = 2$ since $f_n(2) = (2n-1)n$, compare (2.23). In particular, (2.24) confirms that indeed the last digit in the column for $s = 10$ is always n mod 10—an observation from Table 2.1. $\diamondsuit$

Remark 2.2.7. The integers $f_3(k)$ (respectively $f_4(k)$) also arise in physics, see for instance [BBBG08], and are referred to as *hexagonal* (respectively *diamond*) *lattice integers*. The corresponding entries in Sloane's online encyclopedia [Slo09] are `A002893` and `A002895`. We recall the following formulae [BBBG08, (186)–(188)], relating these sequences in non-obvious ways:

$$\begin{aligned}\left(\sum_{k\geqslant 0} f_3(k)(-x)^k\right)^2 &= \sum_{k\geqslant 0} f_2(k)^3 \frac{x^{3k}}{((1+x)^3(1+9x))^{k+\frac{1}{2}}} \\ &= \sum_{k\geqslant 0} f_2(k) f_3(k) \frac{(-x(1+x)(1+9x))^k}{((1-3x)(1+3x))^{2k+1}} \\ &= \sum_{k\geqslant 0} f_4(k) \frac{x^k}{((1+x)(1+9x))^{k+1}}.\end{aligned}$$

It would be instructive to similarly engage $f_5(k)$ for which we have

$$f_5(k) = \binom{2\,k}{k} \sum_{j=0}^{k} \frac{\binom{k}{j}^4}{\binom{2\,k}{2\,j}}\, {}_3F_2\left(\begin{matrix} -j, -j, -j \\ 1, \frac{1}{2} - j \end{matrix} \middle| \frac{1}{4}\right),$$

as follows from (2.11). $\diamondsuit$

2.3 Analytic features of the moments

This section collects analytic features of the moments $W_n(s)$ as a function in s. In particular, it is shown that the recurrences for the even moments $W_n(2k)$, described in Section 2.2, extend to functional equations. This is deduced in the usual way from Carlson's theorem. Still we find it instructive to give the details, especially as the explicit form of the functional equations and the resulting pole structures were crucial for discovery and proof of the closed forms in the cases $n = 3, 4, 5$ obtained in here and in [BSW11, BSWZ11], as was true for the results in Section 2.2.

2.3.1 Analyticity

We start with a preliminary investigation of the analyticity of $W_n(s)$ for a given n. This analyticity also follows from the general principle that the moment functions of bounded random variables are always analytic in a strip of the complex plane containing the right half-plane—but again we prefer to give a short direct proof.

Proposition 2.3.1. *$W_n(s)$ is analytic at least for* $\operatorname{Re} s > 0$.

Proof. Let s_0 be a real number such that the integral in (2.1) converges for $s = s_0$. Then we claim that $W_n(s)$ is analytic in s for $\operatorname{Re} s > s_0$. To this end, let s be such that $s_0 < \text{Re } s \leqslant s_0 + \lambda$ for some real $\lambda > 0$. For any real $0 \leqslant a \leqslant n$,

$$|a^s| = a^{\text{Re } s} \leqslant n^\lambda a^{s_0},$$

and therefore

$$\sup_{s_0 < \text{Re } s \leqslant s_0+\lambda} \int_{[0,1]^n} \left| \left| \sum_{k=1}^n e^{2\pi \mathrm{i} x_k} \right|^s \right| \mathrm{d}\boldsymbol{x} \leqslant n^\lambda W_n(s_0) < \infty.$$

This local boundedness implies, see for instance [Mat01], that $W_n(s)$ as defined by the integral in (2.1) is analytic in s for Re $s > s_0$. Since the integral clearly converges for $s = 0$, the claim follows. $\square$

This result will be extended in Theorem 2.3.5 and Corollary 2.3.6.

2.3.2 $n = 1$ and $n = 2$

It follows straight from the integral definition (2.1) that $W_1(s) = 1$. In the case $n = 2$, direct integration of (2.40) with $n = 2$ yields

$$W_2(s) = 2^{s+1} \int_0^{1/2} \cos(\pi t)^s \mathrm{d}t = \binom{s}{s/2}, \tag{2.25}$$

which may also be obtained using (2.9). In particular, $W_2(1) = 4/\pi$. It may be worth noting that neither *Maple* 14 nor *Mathematica* 7 can evaluate $W_2(1)$ if it is entered naively in form of the defining (2.1) (or expanded as the square root of a sum of squares), each returning the symbolic answer ‘0’.

2.3.3 Functional equations

We may lift the recursive structure of f_n, defined in Section 2.2, to W_n to a fair degree on appealing to Carlson's theorem [Tit39, 5.81]. We recall that a function f is of *exponential type* in a region if $|f(z)| \leqslant M e^{c|z|}$ for some constants M and c.

Theorem 2.3.2 (Carlson)**.** *Let f be analytic in the right half-plane $\operatorname{Re} z \geqslant 0$ and of exponential type with the additional requirement that*

$$|f(z)| \leqslant M e^{d|z|}$$

for some $d < \pi$ on the imaginary axis $\operatorname{Re} z = 0$. If $f(k) = 0$ for $k = 0, 1, 2, \ldots$ then $f(z) = 0$ identically.

Theorem 2.3.3. *Given that $f_n(k)$ satisfies a recurrence*

$$c_{n,0}(k) f_n(k) + \cdots + c_{n,\lambda}(k) f_n(k + \lambda) = 0$$

with polynomial coefficients $c_{n,j}(k)$ (see Theorem 2.2.4) then $W_n(s)$ satisfies the corresponding functional equation

$$c_{n,0}(s/2) W_n(s) + \cdots + c_{n,\lambda}(s/2) W_n(s + 2\lambda) = 0,$$

for $\operatorname{Re} s \geqslant 0$.

Proof. Let

$$U_n(s) := c_{n,0}(s) W_n(2s) + \cdots + c_{n,\lambda}(s) W_n(2s + 2\lambda).$$

Since $f_n(k) = W_n(2k)$ by Proposition 2.2.1, $U_n(s)$ vanishes at the nonnegative integers by assumption. Consequently, $U_n(s)$ is zero throughout the right half-plane and we are done—once we confirm that Theorem 2.3.2 applies. By Proposition 2.3.1, $W_n(s)$

is analytic for Re $s \geqslant 0$. Clearly, $|W_n(s)| \leqslant n^{\mathrm{Re}\, s}$. Thus

$$|U_n(s)| \leqslant \left(|c_{n,0}(s)| + |c_{n,1}(s)|n^2 + \cdots + |c_{n,\lambda}(s)|n^{2\lambda}\right) n^{2\,\mathrm{Re}\, s}.$$

In particular, $U_n(s)$ is of exponential type. Further, $U_n(s)$ is polynomially bounded on the imaginary axis Re $s = 0$. Thus U_n satisfies the growth conditions of Theorem 2.3.2. □

Example 2.3.4. For $n = 2, 3, 4, 5$ we find

$$\begin{aligned}
(s+2)W_2(s+2) - 4(s+1)W_2(s) &= 0,\\
(s+4)^2W_3(s+4) - 2(5s^2+30s+46)W_3(s+2) + 9(s+2)^2W_3(s) &= 0,\\
(s+4)^3W_4(s+4) - 4(s+3)(5s^2+30s+48)W_4(s+2) + 64(s+2)^3W_4(s) &= 0,
\end{aligned}$$

and

$$\begin{aligned}
(s+6)^4W_5(s+6) - (35(s+5)^4 + 42(s+5)^2 + 3)W_5(s+4)\ \ +&\\
(s+4)^2(259(s+4)^2 + 104)W_5(s+2) - 225(s+4)^2(s+2)^2W_5(s) &= 0.
\end{aligned}$$

◊

We note that in each case the recursion lets us determine significant information about the nature and position of any poles of $W_n(s)$. We exploit this in the next theorem for $n \geqslant 3$. The case $n = 2$ is transparent since as determined above $W_2(s) = \binom{s}{s/2}$ which has simple poles at the negative odd integers.

Theorem 2.3.5. *Let an integer $n \geqslant 3$ be given. The recursion guaranteed by Theorem 2.3.3 provides an analytic continuation of $W_n(s)$ to all of the complex plane with poles of at most order two at certain negative integers.*

Proof. Proposition 2.3.1 proves analyticity in the right halfplane. It is clear that the recursion given by Theorem 2.3.3 ensures an analytic continuation with poles only possible at negative integer values compatible with the recursion. Indeed, with $\lambda = \lceil n/2 \rceil$ we have

$$W_n(s) = -\frac{c_{n,1}(s/2)W_n(s+2) + \cdots + c_{n,\lambda}(s/2)W_n(s+2\lambda)}{c_{n,0}(s/2)} \tag{2.26}$$

with the $c_{n,j}$ as in (2.16). We observe that the right side of (2.26) only involves $W_n(s+2k)$ for $k \geqslant 1$. Therefore the least negative pole can only occur at a zero of $c_{n,0}(s/2)$ which is explicitly given in (2.17). We then note that the recursion forces poles to be simple or of order two, and to be replicated as claimed. □

Corollary 2.3.6. *If* $n \geqslant 3$ *then* $W_n(s)$*, as given by* (2.1)*, is analytic for* $\operatorname{Re} s > -2$.

Proof. This follows directly from Theorem 2.3.5, the fact that $c_{n,0}(s/2)$ given in (2.17) has no zero for $s = -1$, and the proof of Proposition 2.3.1. □

In Figure 2.3, on page 18, the analytic continuations for each of W_3, W_4, W_5, and W_6 are plotted on the real line.

Example 2.3.7. Using the recurrence given in Example 2.3.4 we find that $W_3(s)$ has simple poles at $s = -2, -4, -6, \ldots$, compare Figure 2.3(a). Moreover, the residue at $s = -2$ is given by $\operatorname{Res}_{-2}(W_3) = 2/(\sqrt{3}\pi)$, and all other residues of W_3 are rational multiples thereof. This may be obtained from the integral representation given in (2.29) observing that, at s a negative even integer, the residue contributions are entirely from the first term. ◊

Example 2.3.8. Similarly, we find that W_4 has double poles at $-2, -4, -6, \ldots$, compare Figure 2.3(b). With more work, or using a more sophisticated analysis as in

[BSWZ11], it is possible to show that

$$\lim_{s\to-2}(s+2)^2\,W_4(s)=\frac{3}{2\pi^2},$$

and in similar fashion the complete structure of $W_4(s)$ is thus accessible. $\Diamond$

Remark 2.3.9. More generally, it would appear that Theorem 2.3.5 can be extended to show that

- for n odd W_n has simple poles at $-2p$ for $p=1,2,3,\ldots$, while
- for n even W_n has simple poles at $-2p$ and $2(1-p)-n/2$ for $p=1,2,3,\ldots$ which will overlap when $4|n$.

This conjecture is further investigated in [BSW11]. $\Diamond$

We close this section by remarking that the knowledge about the poles of W_n for instance reveals the asymptotic behaviour of the densities p_n at 0. This is detailed in [BSWZ11] where closed forms for the densities are investigated, with particular emphasis on $n=3,4,5$. It is worth noting that p_5 was first proven rigorously not to be linear on $[0,1]$ in [Fet63].

2.3.4 Convolution series

Our attempt to lift the convolution sum (2.11) to $W_n(s)$ resulted in the following conjecture:

Conjecture 2.3.10. *For positive integers n and complex s,*

$$W_{2n}(s)\stackrel{?}{=}\sum_{j\geqslant 0}\binom{s/2}{j}^2 W_{2n-1}(s-2j). \tag{2.27}$$

It is understood that the right-hand side of (2.27) refers to the analytic continuation of W_n as guaranteed by Theorem 2.3.5. Conjecture 2.3.10, which is consistent with the pole structure described in Remark 2.3.9, has been confirmed by David Broadhurst [Bro09] using a Bessel integral representation for W_n, given in (2.28), for $n = 2, 3, 4, 5$ and odd integers $s < 50$ to a precision of 50 digits. By (2.11) the conjecture clearly holds for s an even positive integer. For $n = 1$ it is confirmed next.

Example 2.3.11. For $n = 1$ we obtain from (2.27) using $W_1(s) = 1$,

$$W_2(s) = \sum_{j \geqslant 0} \binom{s/2}{j}^2 = \binom{s}{s/2}$$

which agrees with (2.25). ♢

We remark that a partial resolution of Conjecture 2.3.10 is obtained in [BSWZ11].

2.4 Bessel integral representations

As noted in the introduction, Kluyver [Klu06] made a lovely analysis of the cumulative distribution function of the distance traveled by a "rambler" in the plane for various fixed step lengths. In particular, for our uniform walk Kluyver provides the Bessel function representation

$$P_n(t) = t \int_0^\infty J_1(xt)\, J_0^n(x)\, \mathrm{d}x.$$

Thus, $W_n(s) = \int_0^n t^s\, p_n(t)\, \mathrm{d}t$, where $p_n = P_n'$. From here, Broadhurst [Bro09] obtains

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^k J_0^n(x)\, \mathrm{d}x \tag{2.28}$$

for real s and is valid as long as $2k > s > \max(-2, -\frac{n}{2})$.

Remark 2.4.1. For $n = 3, 4$, symbolic integration in *Mathematica* of (2.28) leads to interesting analytic continuations [Cra09] such as

$$W_3(s) = \frac{1}{2^{2s+1}} \tan\left(\frac{\pi s}{2}\right) \binom{s}{\frac{s-1}{2}}^2 {}_3F_2\left(\left.\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{s+3}{2}, \frac{s+3}{2}\end{matrix}\right| \frac{1}{4}\right) + \binom{s}{\frac{s}{2}} {}_3F_2\left(\left.\begin{matrix}-\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \\ 1, -\frac{s-1}{2}\end{matrix}\right| \frac{1}{4}\right), \tag{2.29}$$

and

$$W_4(s) = \frac{1}{2^{2s}} \tan\left(\frac{\pi s}{2}\right) \binom{s}{\frac{s-1}{2}}^3 {}_4F_3\left(\left.\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{s}{2}+1 \\ \frac{s+3}{2}, \frac{s+3}{2}, \frac{s+3}{2}\end{matrix}\right| 1\right) + \binom{s}{\frac{s}{2}} {}_4F_3\left(\left.\begin{matrix}\frac{1}{2}, -\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \\ 1, 1, -\frac{s-1}{2}\end{matrix}\right| 1\right). \tag{2.30}$$

We note that for $s = 2k = 0, 2, 4, \ldots$ the first term in (2.29) (resp. (2.30)) is zero and the second is a formula given in (2.12) (resp. (2.13)). Thence, one can in principle prove (2.29) and (2.30) by applying Carlson's theorem—after showing the singularities at $1, 3, 5, \ldots$ are removable. A rigorous proof, along with extensions and more details, appears in [BSW11]. $\diamondsuit$

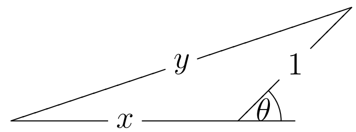
2.5 The odd moments of a three-step walk

In this section, we combine the results of the previous sections to finally prove the hypergeometric evaluation (2.6) of the moments $W_3(k)$ in Theorem 2.5.1.

It is elementary to express the distance y of an $(n+1)$-step walk conditioned on a given distance x of an n-step walk. By a simple application of the cosine rule we find

$$y^2 = x^2 + 1 + 2x\cos(\theta),$$

where θ is the outside angle of the triangle with sides of lengths x, 1, and y:



It follows that the s-th moment of an $(n+1)$-step walk conditioned on a given distance x of an n-step walk is

$$g_s(x) := \frac{1}{\pi}\int_0^\pi y^s \,\mathrm{d}\theta = |x-1|^s \,{}_2F_1\left(\begin{matrix}\frac{1}{2}, -\frac{s}{2} \\ 1\end{matrix}\middle| -\frac{4x}{(x-1)^2}\right). \tag{2.31}$$

Here we appealed to symmetry to restrict the angle to $\theta \in [0, \pi)$. We then evaluated the integral in hypergeometric form which, for instance, can be done with the help of *Mathematica*. Observe that $g_s(x)$ does not depend on n. Since $W_{n+1}(s)$ is the s-th moment of the distance of an $(n+1)$-step walk, we obtain

$$W_{n+1}(s) = \int_0^n g_s(x)\, p_n(x)\,\mathrm{d}x, \tag{2.32}$$

where $p_n(x)$ is the density of the distance x for an n-step walk. Clearly, for the 1-step walk we have $p_1(x) = \delta_1(x)$, a Dirac delta function at $x = 1$. It is also easily shown that the probability density for a 2-step walk is given by $p_2(x) = 2(\pi\sqrt{4-x^2})^{-1}$ for $0 \leqslant x \leqslant 2$ and 0 otherwise. The density $p_3(x)$ is given in (2.3).

For $n = 3$, based on (2.12) we define

$$V_3(s) := {}_3F_2\left(\begin{matrix}\frac{1}{2}, -\frac{s}{2}, -\frac{s}{2} \\ 1, 1\end{matrix}\middle| 4\right), \tag{2.33}$$

so that by Proposition 2.2.1 and (2.12), $W_3(2k) = V_3(2k)$ for nonnegative integers k. This led us to explore $V_3(s)$ more generally numerically and so to conjecture and eventually prove the following:

Theorem 2.5.1. *For nonnegative even integers and all odd integers k:*

$$W_3(k) = \mathrm{Re}\ V_3(k).$$

Remark 2.5.2. Note that, for all complex s, the function $V_3(s)$ also satisfies the recursion given in Example 2.3.4 for $W_3(s)$—as is routine to prove symbolically using for instance creative telescoping [PWZ96]. However, V_3 does not satisfy the growth conditions of Carlson's Theorem (Theorem 2.3.2). Thus, it yields a rather nice illustration that the hypotheses can fail. $\Diamond$

Proof of Theorem 2.5.1. It remains to prove the result for odd integers. Since, as noted in Remark 2.5.2, for all complex s, the function $V_3(s)$ defined in (2.33) also satisfies the recursion given in Example 2.3.4, it suffices to show that the values given for $s = 1$ and $s = -1$ are correct. From (2.32), we have the following expression for W_3:

$$W_3(s) = \frac{2}{\pi}\int_0^2 \frac{g_s(x)}{\sqrt{4-x^2}}\mathrm{d}x = \frac{2}{\pi}\int_0^{\pi/2} g_s(2\sin(t))\mathrm{d}t. \tag{2.34}$$

For $s = 1$: equation (2.31), [BB98, Exercise 1c, p. 16], and Jacobi's imaginary transformations [BB98, Exercises 7a) & 8b), p. 73] allow us to write

$$\frac{\pi}{2}\, g_1(x) = (x+1)E\left(\frac{2\sqrt{x}}{x+1}\right) = \mathrm{Re}\ \big(2E(x) - (1-x^2)K(x)\big) \tag{2.35}$$

where $K(k) = \int_0^{\pi/2} \mathrm{d}t/\sqrt{1-k^2\sin^2(t)}$ and $E(k) = \int_0^{\pi/2} \sqrt{1-k^2\sin^2(t)}\,\mathrm{d}t$ denote the complete elliptic integrals of the first and second kind. Thus, from (2.34) and (2.35),

$$\begin{aligned}
W_3(1) &= \frac{4}{\pi^2}\,\mathrm{Re}\int_0^{\pi/2}\Big(2\,E(2\sin(t)) - (1-4\sin^2(t))K(2\sin(t))\Big)\,\mathrm{d}t \\
&= \frac{4}{\pi^2}\,\mathrm{Re}\int_0^{\pi/2}\int_0^{\pi/2} 2\sqrt{1-4\sin^2(t)\sin^2(r)}\,\mathrm{d}t\mathrm{d}r \\
&\quad - \frac{4}{\pi^2}\,\mathrm{Re}\int_0^{\pi/2}\int_0^{\pi/2} \frac{1-4\sin^2(t)}{\sqrt{1-4\sin^2(t)\sin^2(r)}}\,\mathrm{d}t\mathrm{d}r.
\end{aligned}$$

Amalgamating the two last integrals and parameterizing, we consider

$$Q(a) := \frac{4}{\pi^2}\int_0^{\pi/2}\int_0^{\pi/2} \frac{1+a^2\sin^2(t) - 2\,a^2\sin^2(t)\sin^2(r)}{\sqrt{1-a^2\sin^2(t)\sin^2(r)}}\,\mathrm{d}t\mathrm{d}r. \tag{2.36}$$

We now use the binomial theorem to integrate (2.36) term-by-term for $|a| < 1$ and substitute $\frac{2}{\pi}\int_0^{\pi/2}\sin^{2m}(t)\,\mathrm{d}t = (-1)^m\binom{-1/2}{m}$ throughout. Moreover, $(-1)^m\binom{-\alpha}{m} = (\alpha)_m/m!$ where the later denotes the *Pochhammer* symbol. Evaluation of the consequent infinite sum produces:

$$\begin{aligned}
Q(a) &= \sum_{k\geqslant 0}(-1)^k\binom{-1/2}{k}\left(a^{2k}\binom{-1/2}{k}^2 - a^{2k+2}\binom{-1/2}{k}\binom{-1/2}{k+1} - 2a^{2k+2}\binom{-1/2}{k+1}^2\right) \\
&= \sum_{k\geqslant 0}(-1)^k a^{2k}\binom{-1/2}{k}^3\frac{1}{(1-2k)^2} \\
&= {}_3F_2\left(\left.{-\tfrac12, -\tfrac12, \tfrac12 \atop 1, 1}\right| a^2\right).
\end{aligned}$$

Analytic continuation to $a = 2$ yields the claimed result as per for $s = 1$.

For $s=-1$**:** we similarly and more easily use (2.31) and (2.34) to derive

$$\begin{aligned} W_3(-1) &= \operatorname{Re}\,\frac{4}{\pi^2}\int_0^{\pi/2} K(2\sin(t))\,\mathrm{d}t \\ &= \operatorname{Re}\,\frac{4}{\pi^2}\int_0^{\pi/2}\int_0^{\pi/2}\frac{1}{\sqrt{1-4\sin^2(t)\sin^2(r)}}\,\mathrm{d}t\mathrm{d}r = V_3(-1). \end{aligned}$$

$\square$

Example 2.5.3. Theorem 2.5.1 allows us to establish the following equivalent expressions for $W_3(1)$:

$$\begin{aligned} W_3(1) &= \frac{4\sqrt{3}}{3}\left({}_3F_2\left(\left.{-\frac{1}{2},-\frac{1}{2},-\frac{1}{2} \atop 1,1}\right|\frac{1}{4}\right)-\frac{1}{\pi}\right)+\frac{\sqrt{3}}{24}\,{}_3F_2\left(\left.{\frac{1}{2},\frac{1}{2},\frac{1}{2} \atop 2,2}\right|\frac{1}{4}\right) \\ &= 2\sqrt{3}\,\frac{K^2\left(k_3\right)}{\pi^2}+\sqrt{3}\,\frac{1}{K^2\left(k_3\right)} \\ &= \frac{3}{16}\frac{2^{1/3}}{\pi^4}\Gamma^6\left(\frac{1}{3}\right)+\frac{27}{4}\frac{2^{2/3}}{\pi^4}\Gamma^6\left(\frac{2}{3}\right). \end{aligned}$$

These rely on using Legendre's identity and several Clausen-like product formulae, plus Legendre's evaluation of $K(k_3)$ where $k_3 := \frac{\sqrt{3}-1}{2\sqrt{2}}$ is the *third singular value* as in [BB98]. More simply but similarly, we have

$$W_3(-1) = 2\sqrt{3}\,\frac{K^2\left(k_3\right)}{\pi^2} = \frac{3}{16}\frac{2^{1/3}}{\pi^4}\,\Gamma^6\left(\frac{1}{3}\right).$$

Using the recurrence presented in Example 2.3.4 it follows that similar expressions can be given for W_3 evaluated at odd integers.

In [BSW11], corresponding hypergeometric closed forms for W_4 are presented. $\diamondsuit$

2.6 Appendix

2.6.1 An alternative proof of the series evaluation (2.9)

We begin with:

Proposition 2.6.1. *For complex s with* $\operatorname{Re} s \geqslant 0$,

$$W_n(s) = n^s \sum_{m \geqslant 0} (-1)^m \binom{s/2}{m} \left(\frac{2}{n}\right)^{2m} \int_{[0,1]^n} \left(\sum_{1 \leqslant i < j \leqslant n} \sin^2(\pi(x_j - x_i)) \right)^m \mathrm{d}\boldsymbol{x}. \quad (2.37)$$

Proof. Start with

$$\begin{aligned}
\left| \sum_{k=1}^n e^{2\pi \mathrm{i} x_k} \right|^2 &= \left(\sum_{k=1}^n \cos(2\pi x_k) \right)^2 + \left(\sum_{k=1}^n \sin(2\pi x_k) \right)^2 \\
&= \left(\sum_{i<j} \Big(\cos(2\pi x_i) + \cos(2\pi x_j) \Big)^2 + \Big(\sin(2\pi x_i) + \sin(2\pi x_j) \Big)^2 \right) - n(n-2) \\
&= 4 \left(\sum_{i<j} \cos^2(\pi(x_j - x_i)) \right) - n(n-2) \\
&= n^2 - 4 \left(\sum_{i<j} \sin^2(\pi(x_j - x_i)) \right).
\end{aligned}$$

Therefore, noting that binomial expansion may be applied to the integrand outside a set of n-dimensional measure zero,

$$\begin{aligned}
W_n(s) &= \int_{[0,1]^n} \left(n^2 - 4 \left(\sum_{i<j} \sin^2(\pi(x_j - x_i)) \right) \right)^{s/2} \mathrm{d}\boldsymbol{x} \\
&= n^s \int_{[0,1]^n} \sum_{m \geqslant 0} (-1)^m \binom{s/2}{m} \left(\frac{2}{n}\right)^{2m} \left(\sum_{i<j} \sin^2(\pi(x_j - x_i)) \right)^m \mathrm{d}\boldsymbol{x}.
\end{aligned}$$

Thus the result follows once changing the order of integration and summation is justified. Observe that if s is real then $(-1)^m \binom{s/2}{m}$ has a fixed sign for $m > s/2$ and we can apply monotone convergence. On the other hand, if s is complex then we may use

$$\lim_{m\to\infty} \left| \frac{\binom{s/2}{m}}{\binom{\operatorname{Re} s/2}{m}} \right| = \left| \frac{\Gamma(-\operatorname{Re} s/2)}{\Gamma(-s/2)} \right|,$$

which follows from Stirling's approximation, and apply dominated convergence using the real case for comparison. □

We next evaluate the integrals in (2.37):

Theorem 2.6.2. *For nonnegative integers m,*

$$\int_{[0,1]^n} \left(\sum_{i<j} \sin^2(\pi(x_j - x_i)) \right)^m \mathrm{d}\boldsymbol{x} = \left(\frac{n}{2}\right)^{2m} \sum_{k=0}^{m} \frac{(-1)^k}{n^{2k}} \binom{m}{k} \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2.$$

Proof. Denote the left-hand by $I_{n,m}$. As in the proof of Proposition 2.2.1 we note that the claim is equivalent to asserting that $2^{2m} I_{n,m}$ is the constant term of

$$(n^2 - (x_1 + \cdots + x_n)(1/x_1 + \cdots + 1/x_n))^m.$$

Observe that

$$\begin{aligned}(n^2 - (x_1 + \cdots + x_n)(1/x_1 + \cdots + 1/x_n))^m &= \left(\sum_{1\leqslant i<j\leqslant n} \left(2 - \frac{x_i}{x_j} - \frac{x_j}{x_i} \right) \right)^m \\ &= (-1)^m \left(\sum_{1\leqslant i<j\leqslant n} \frac{(x_j - x_i)^2}{x_i x_j} \right)^m.\end{aligned}$$

The result therefore follows from the next proposition. □

As before, we denote by 'ct' the operator which extracts from an expression the constant term of its Laurent expansion.

Proposition 2.6.3. *For any integers $1 \leqslant i_1 \neq j_1, \ldots, i_m \neq j_m \leqslant n$,*

$$\int_{[0,1]^n} \prod_{k=1}^{m} 4\sin^2(\pi(x_{j_k} - x_{i_k}))\, \mathrm{d}\boldsymbol{x} = (-1)^m \operatorname{ct} \prod_{k=1}^{m} \frac{(x_{j_k} - x_{i_k})^2}{x_{i_k} x_{j_k}}.$$

Proof. We prove this by evaluating both sides independently. First, we have

$$\begin{aligned}
\mathrm{LHS} &:= \int_{[0,1]^n} \prod_{k=1}^{m} 4\sin^2(\pi(x_{j_k} - x_{i_k}))\,\mathrm{d}\boldsymbol{x} \\
&= (-1)^m \int_{[0,1]^n} \prod_{k=1}^{m} \left(e^{\pi \mathrm{i}(x_{j_k} - x_{i_k})} - e^{-\pi \mathrm{i}(x_{j_k} - x_{i_k})}\right)^2 \mathrm{d}\boldsymbol{x} \\
&= (-1)^m \sum_{\boldsymbol{a},\boldsymbol{b}} (-1)^{\sum_k (a_k + b_k - 2)/2} \int_{[0,1]^n} e^{\pi \mathrm{i} \sum_k (a_k + b_k)(x_{j_k} - x_{i_k})}\,\mathrm{d}\boldsymbol{x} \\
&= \sum_{\boldsymbol{a},\boldsymbol{b}} (-1)^{\sum_k (a_k + b_k)/2} \int_{[0,1]^n} \cos\left(\pi \sum_k (a_k + b_k)(x_{j_k} - x_{i_k})\right) \mathrm{d}\boldsymbol{x}
\end{aligned}$$

where the last two sums are over all sequences $\boldsymbol{a}, \boldsymbol{b} \in \{\pm 1\}^m$. In the last step the summands corresponding to $(\boldsymbol{a}, \boldsymbol{b})$ and $(-\boldsymbol{a}, -\boldsymbol{b})$ have been combined.

Now note that, for a an even integer,

$$\int_0^1 \cos(\pi(ax + b))\mathrm{d}x = \begin{cases} \cos(\pi b) & \text{if } a = 0, \\ 0 & \text{otherwise.} \end{cases} \tag{2.38}$$

Since $a_k + b_k$ is even, we may apply (2.38) iteratively to obtain

$$\int_{[0,1]^n} \cos\left(\pi \sum_k (a_k + b_k)(x_{j_k} - x_{i_k})\right) \mathrm{d}\boldsymbol{x} = \begin{cases} 1 & \text{if } \boldsymbol{a}, \boldsymbol{b} \in S, \\ 0 & \text{otherwise,} \end{cases}$$

where S denotes the set of sequences $\boldsymbol{a}, \boldsymbol{b} \in \{\pm 1\}^m$ such that

$$\sum_{k=1}^{m} (a_k + b_k)(x_{j_k} - x_{i_k}) = 0$$

as a polynomial in $\boldsymbol{x}$. It follows that

$$\mathrm{LHS} = \sum_{\boldsymbol{a},\boldsymbol{b} \in S} (-1)^{\sum_k (a_k + b_k)/2} \tag{2.39}$$

On the other hand, consider

$$\mathrm{RHS} := (-1)^m \operatorname{ct} \prod_{k=1}^{m} \frac{(x_{j_k} - x_{i_k})^2}{x_{i_k} x_{j_k}},$$

and observe that, by a similar argument as above,

$$(-1)^m \prod_{k=1}^{m} \frac{(x_{j_k} - x_{i_k})^2}{x_{i_k} x_{j_k}} = \sum_{\boldsymbol{a},\boldsymbol{b}} \prod_{k=1}^{m} (-1)^{(a_k+b_k)/2} \left(\frac{x_{j_k}}{x_{i_k}}\right)^{(a_k+b_k)/2}$$

where the sum is again over all sequences $\boldsymbol{a}, \boldsymbol{b} \in \{\pm 1\}^m$. From here, it is straightforward to verify that RHS is equivalent to the expression given for LHS in (2.39). $\square$

The desired evaluation is now available. On combining Theorem 2.6.2 and Proposition 2.6.1 we obtain that for $\operatorname{Re} s \geqslant 0$,

$$W_n(s) = n^s \sum_{m \geqslant 0} (-1)^m \binom{s/2}{m} \sum_{k=0}^{m} \frac{(-1)^k}{n^{2k}} \binom{m}{k} \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2.$$

This is (2.9).

Remark 2.6.4. We briefly outline the experimental genesis of the evaluation given in Proposition 2.2.1. The sequence $2^{2m} I_{3,m}$ appearing in the proof of Theorem 2.6.2 is Sloane's, [Slo09], `A093388` where a link to [Ver99] is given. That paper contains the sum

$$2^{2m} I_{3,m} = (-1)^m \sum_{k=0}^{m} \binom{m}{k} (-8)^k \sum_{j=0}^{m-k} \binom{m-k}{j}^3$$

and further mentions that $2^{2m} I_{3,m}$ is therefore the coefficient of $(xyz)^m$ in

$$(8xyz - (x+y)(y+z)(z+x))^m.$$

Observe also that $2^{2m} I_{2,m}$ is the coefficient of $(xy)^m$ in

$$(4xy - (x+y)(y+x))^m.$$

It was then noted that

$$8xyz - (x+y)(y+z)(z+x) = 3^2 xyz - (x+y+z)(xy+yz+zx)$$

and this line of extrapolation led to the correct conjecture, so that the next case would involve

$$4^2 wxyz - (w+x+y+z)(wxy+xyz+yzw+zwx),$$

which was what we have now proven. $\Diamond$

2.6.2 Numerical evaluations

A one-dimensional reduction of the integral (2.1) may be achieved by taking periodicity into account:

$$W_n(s) = \int_{[0,1]^{n-1}} \left| 1 + \sum_{k=1}^{n-1} e^{2\pi i x_k} \right|^s \mathrm{d}(x_1, \ldots, x_{n-1}). \tag{2.40}$$

From here, we note that quick and rough estimates are easily obtained using the *Monte Carlo* method. Moreover, since the integrand function is periodic this seems like an invitation to use lattice sequences—a *quasi-Monte Carlo* method. E.g., the lattice sequence from [CKN06] can be straightforwardly employed to calculate an entire table in one run by keeping a running sum over different values of n and s. A standard stochastic error estimator can then be obtained by random shifting.

Generally, however, Broadhurst's representation (2.28) seems to be the best available for high precision evaluations of $W_n(s)$. We close by commenting on the special cases $n = 3, 4$.

Example 2.6.5. The first high precision evaluations of W_3 were performed by David Bailey who confirmed the initially only conjectured Theorem 2.5.1 for $s = 2, \ldots, 7$ to 175 digits. This was done on a 256-core LBNL system in roughly 15 minutes by applying tanh-sinh integration to

$$W_3(s) = \int_0^1 \int_0^1 \left(9 - 4(\sin^2(\pi x) + \sin^2(\pi y) + \sin^2(\pi(x-y)))\right)^{s/2} \,\mathrm{d}y\mathrm{d}x,$$

which is obtained from (2.40) as in Proposition 2.6.1. More practical is the one-dimensional form (2.34) which can deliver high precision results in minutes on a simple laptop. For integral s, Theorem 2.5.1 allows extremely high precision evaluations. $\Diamond$

Example 2.6.6. Assuming that Conjecture 2.3.10 holds for $n = 2$ (for a proof, see [BSWZ11]), Theorem 2.5.1 implies that for nonnegative integers k

$$W_4(k) \stackrel{?}{=} \mathrm{Re} \sum_{j \geqslant 0} \binom{s/2}{j}^2 {}_3F_2\left(\left. \begin{matrix} \frac{1}{2}, -\frac{k}{2}+j, -\frac{k}{2}+j \\ 1, 1 \end{matrix} \right| 4 \right).$$

This representation is very suitable for high precision evaluations of W_4 since, roughly, one correct digit is added by each term of the sum. Formula (2.30) by Crandall also lends itself quite well for numerical work (by slightly perturbing even s for integer arguments). $\Diamond$

Chapter 3

Three-step and four-step random walk integrals

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[BSW11] *Three-step and four-step random walk integrals*
(with Jonathan M. Borwein, James Wan)
to appear in Experimental Mathematics

Abstract We investigate the moments of 3-step and 4-step uniform random walks in the plane. In particular, we further analyse a formula conjectured in [BNSW11] expressing 4-step moments in terms of 3-step moments. Diverse related results including hypergeometric and elliptic closed forms for $W_4(\pm 1)$ are given and two new conjectures are recorded.

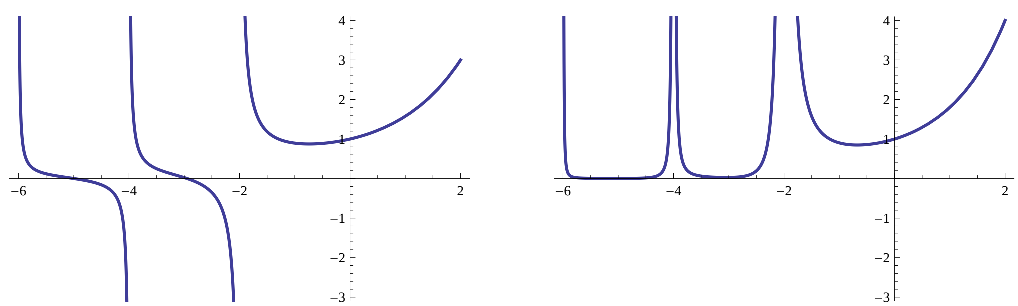
3.1 Introduction and preliminaries

Continuing research commenced in [BNSW11], for complex s, we consider the n-dimensional integral

$$W_n(s) := \int_{[0,1]^n} \left| \sum_{k=1}^{n} e^{2\pi x_k i} \right|^s \mathrm{d}\boldsymbol{x} \tag{3.1}$$

which occurs in the theory of uniform random walks in the plane, where at each step a unit-step is taken in a random direction. As such, the integral (3.1) expresses the s-th moment of the distance to the origin after n steps. The study of such walks largely originated with Pearson more than a century ago [Pea05a, Pea05b]. In his honor we might call such integrals *ramble integrals*, as he posed such questions for a walker or rambler. As discussed in [BNSW11], and illustrated further herein, such ramble integrals are approachable by a mixture of analytic, combinatoric, algebraic and probabilistic methods. They provide interesting numeric and symbolic computation challenges. Indeed, nearly all of our results were discovered experimentally.

For $n \geqslant 3$, the integral (3.1) is well-defined and analytic for $\operatorname{Re} s > -2$, and admits an interesting analytic continuation to the complex plane with poles at certain negative integers, see [BNSW11]. We shall also write W_n for these continuations. In Figure 3.1 we show the continuations of W_3 and W_4 on the negative real axis. Observe the poles of W_3 and W_4 at negative even integers (but note that neither function has zeroes at negative odd integers even though the graphs may suggest otherwise).



(a) W_3 (b) W_4

Figure 3.1: W_3, W_4 analytically continued to the real line.

It is easy to determine that $W_1(s) = 1$, and $W_2(s) = \binom{s}{s/2}$. Furthermore, it is proven in [BNSW11] that, for k a nonnegative integer, in terms of the generalized hypergeometric function, we have

$$W_3(k) = \operatorname{Re}\ {}_3F_2\left(\left.{\frac{1}{2}, -\frac{k}{2}, -\frac{k}{2} \atop 1, 1}\right| 4\right). \tag{3.2}$$

From here, the following expressions for $W_3(1)$ can be established:

$$\begin{aligned} W_3(1) &= \frac{4\sqrt{3}}{3}\left({}_3F_2\left(\left.{-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \atop 1, 1}\right| \frac{1}{4}\right) - \frac{1}{\pi}\right) + \frac{\sqrt{3}}{24}{}_3F_2\left(\left.{\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop 2, 2}\right| \frac{1}{4}\right) && (3.3) \\ &= 2\sqrt{3}\,\frac{K^2(k_3)}{\pi^2} + \sqrt{3}\,\frac{1}{K^2(k_3)} && (3.4) \\ &= \frac{3}{16}\frac{2^{1/3}}{\pi^4}\Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4}\frac{2^{2/3}}{\pi^4}\Gamma^6\left(\frac{2}{3}\right) && (3.5) \\ &= \frac{1}{\pi^2}\left(\frac{2^{1/3}}{4}\beta^2\left(\frac{1}{3}\right) + 2^{2/3}\beta^2\left(\frac{2}{3}\right)\right), && (3.6) \end{aligned}$$

where K is the complete elliptic integral of the first kind, $k_3 := \frac{\sqrt{3}-1}{2\sqrt{2}}$ is the *third singular value* as in [BB98], and $\beta(x) := B(x,x)$ is a central Beta-function value. More simply, but similarly,

$$W_3(-1) = 2\sqrt{3}\,\frac{K^2(k_3)}{\pi^2} = \frac{3}{16}\frac{2^{1/3}}{\pi^4}\,\Gamma^6\left(\frac{1}{3}\right) = \frac{2^{\frac{1}{3}}}{4\pi^2}\beta^2\left(\frac{1}{3}\right). \tag{3.7}$$

Using the two-term recurrence for W_3 given in [BNSW11], it follows that similar expressions can be given for W_3 evaluated at any odd integer. It is one of the goals of this paper to give similar evaluations for a 4-step walk.

For s an even positive integer, the moments $W_n(s)$ take explicit integer values. In fact, for integers $k \geqslant 0$,

$$W_n(2k) = \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2. \tag{3.8}$$

Based on the combinatorial properties of this evaluation, the following conjecture was made in [BNSW11]. Note that the case $n = 1$ is easily resolved.

Conjecture 3.1.1. *For positive integers n and complex s,*

$$W_{2n}(s) \overset{?[1]}{=} \sum_{j\geqslant 0} \binom{s/2}{j}^2 W_{2n-1}(s-2j). \tag{3.9}$$

We investigate this conjecture in some detail in Section 3.4. For $n = 2$, in conjunction with (3.3) this leads to a very efficient computation of W_4 at integers, yielding roughly a digit per term.

3.2 Bessel integral representations

We start with the result of Kluyver [Klu06], amplified in [Wat41, §31.48] and exploited in [BNSW11], to the effect that the probability that an n-step walk ends up within a disc of radius α is

$$P_n(\alpha) = \alpha \int_0^\infty J_1(\alpha x) J_0^n(x)\,\mathrm{d}x. \tag{3.10}$$

From this, David Broadhurst [Bro09] obtains

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^k J_0^n(x)\,\mathrm{d}x \tag{3.11}$$

valid as long as $2k > s > -n/2$. Here and below $J_\nu(z)$ denotes the *Bessel function* of the first kind.

Example 3.2.1 ($W_n(\pm 1)$)**.** In particular, from (3.11), for $n \geqslant 2$, we can write:

$$W_n(-1) = \int_0^\infty J_0^n(x)\,\mathrm{d}x, \quad W_n(1) = n \int_0^\infty J_1(x) J_0(x)^{n-1} \frac{\mathrm{d}x}{x}. \tag{3.12}$$

$\Diamond$

Equation (3.11) enabled Broadhurst to verify Conjecture 3.1.1 for $n = 2, 3, 4, 5$ and odd positive $s < 50$ to a precision of 50 digits. A different proof of (3.11) is outlined in Remark 3.2.3 below. In particular, for $0 < s < n/2$, we have

$$W_n(-s) = 2^{1-s}\frac{\Gamma(1-s/2)}{\Gamma(s/2)}\int_0^\infty x^{s-1}J_0^n(x)\,\mathrm{d}x, \tag{3.13}$$

so that $W_n(-s)$ essentially is (the analytic continuation of) the Mellin transform of the nth power of the Bessel function J_0.

Example 3.2.2. Using (3.13), the evaluations $W_1(s) = 1$ and $W_2(s) = \binom{s}{s/2}$ translate into

$$\begin{aligned}
\int_0^\infty x^{s-1}J_0(x)\,\mathrm{d}x &= 2^{s-1}\frac{\Gamma(s/2)}{\Gamma(1-s/2)},\\
\int_0^\infty x^{s-1}J_0^2(x)\,\mathrm{d}x &= \frac{1}{2\Gamma(1/2)}\frac{\Gamma(s/2)\Gamma(1/2-s/2)}{\Gamma(1-s/2)^2}
\end{aligned}$$

in the region where the left-hand side converges.

The Mellin transforms of J_0^3 and J_0^4 in terms of Meijer G-functions appear in the proofs of Theorems 3.2.7 and 3.2.8. $\Diamond$

Remark 3.2.3. Here, we demonstrate how Ramanujan's "master theorem" may be applied to find the Bessel integral representation (3.11) in a natural way; this and more applications of Ramanujan's master theorem will appear in [AEG+11]. For an alternative proof see [Bro09].

Ramanujan's master theorem [Har78] states that, under certain conditions on the analytic function φ,

$$\int_0^\infty x^{\nu-1}\left(\sum_{k=0}^\infty \frac{(-1)^k}{k!}\varphi(k)x^k\right) = \Gamma(\nu)\varphi(-\nu). \tag{3.14}$$

Based on the evaluation (3.8), we have, as noted in [BNSW11], the generating function

$$\sum_{k\geqslant 0} W_n(2k)\frac{(-x)^k}{(k!)^2} = \left(\sum_{k\geqslant 0}\frac{(-x)^k}{(k!)^2}\right)^n = J_0(2\sqrt{x})^n \tag{3.15}$$

for the even moments. Applying Ramanujan's master theorem (3.14) to $\varphi(k) := W_n(2k)/k!$, we find

$$\Gamma(\nu)\varphi(-\nu) = \int_0^\infty x^{\nu-1} J_0^n(2\sqrt{x})\,\mathrm{d}x. \tag{3.16}$$

Upon a change of variables and setting $s = 2\nu$,

$$W_n(-s) = 2^{1-s}\frac{\Gamma(1-s/2)}{\Gamma(s/2)}\int_0^\infty x^{s-1} J_0^n(x)\,\mathrm{d}x. \tag{3.17}$$

This is the case $k = 0$ of (3.11). The general case follows from the fact that if $F(s)$ is the Mellin transform of $f(x)$, then $(s-2)(s-4)\cdots(s-2k)F(s-2k)$ is the Mellin transform of $\left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^k f(x)$. $\diamondsuit$

3.2.1 Pole structure

A very useful consequence of equation (3.13) is the following proposition.

Proposition 3.2.4 (Poles)**.** *The structure of the poles of W_n is as follows:*

(a) (Reflection) *For $n = 3$, we have explicitly for $k = 0, 1, 2, \ldots$ that*

$$\operatorname{Res}_{(-2k-2)}(W_3) = \frac{2}{\pi\sqrt{3}}\frac{W_3(2k)}{3^{2k}} > 0,$$

and the corresponding poles are simple.

(b) *For each integer $n \geqslant 5$, the function $W_n(s)$ has a simple pole at $-2k-2$ for integers $0 \leqslant k < (n-1)/4$ with residue given by*

$$\operatorname{Res}_{(-2k-2)}(W_n) = \frac{(-1)^k}{2^{2k}(k!)^2} \int_0^\infty x^{2k+1} J_0^n(x)\,\mathrm{d}x. \tag{3.18}$$

(c) *Moreover, for odd $n \geqslant 5$, all poles of $W_n(s)$ are simple as soon as the first $(n-1)/2$ are.*

In fact, we believe that for odd n, all poles of $W_n(s)$ are simple as stated in Conjecture 3.4.1. For individual n this may be verified as in Example 3.2.5. This was done by the authors for $n \leqslant 45$.

Proof. (a) For $n = 3$ it was shown in [BNSW11] that $\operatorname{Res}_{-2}(W_3) = 2/(\sqrt{3}\pi)$. This also follows from (3.24) of Corollary 3.2.9. We remark that from [Wat41, (4) p. 412] this is also the value of the conditional integral $\int_0^\infty x J_0^3(x)\,\mathrm{d}x$ in accordance with (3.18). Letting $r_3(k) := \operatorname{Res}_{(-2k)}(W_n)$, the explicit residue equation is

$$r_3\,(k) = \frac{(10\,k^2 - 30\,k + 23)\,r_3(k-1) - (k-2)^2 r_3(k-2)}{9\,(k-1)^2},$$

which has the asserted solution, when compared to the recursion for $W_3(s)$:

$$(s+4)^2 W_3(s+4) - 2(5s^2 + 30s + 46)W_3(s+2) + 9(s+2)^2 W_3(s) = 0. \tag{3.19}$$

We give another derivation in Example 3.3.4 in Section 3.3.

(b) For $n \geqslant 5$ we note that the integral in (3.18) is absolutely convergent since $|J_0(x)| \leqslant 1$ on the real axis and $J_0(x) \approx \sqrt{2/(\pi x)}\,\cos(x - \pi/4)$ (see [AS72, (9.2.1)]). Since

$$\lim_{s\to 2k}(s-2k)\Gamma(1-s/2) = 2\frac{(-1)^k}{(k-1)!},$$

the residue is as claimed by (3.17).

(c) As shown in [BNSW11] W_n, for odd n, satisfies a recursion of the form

$$(-1)^{\lambda}\,(n!!)^2\prod_{j=1}^{\lambda-1}(s+2j)^2\;W_n(s)+c_1(s)W_n(s+2)+\cdots+(s+2\lambda)^{n-1}\,W_n(s+2\lambda)=0,$$

with polynomial coefficients of degree $n-1$ where $\lambda := (n+1)/2$. From this, on multiplying by $(s+2k)(s+2k-2)\cdots(s-2k+2\lambda)$ one may derive a corresponding recursion for $\mathrm{Res}_{(-2k)}(W_n)$ for $k = 1, 2, \ldots$ Inductively, this lets us establish that the poles are simple. The argument breaks down if one of the initial values is infinite as it is when $4|n$.

$\square$

Example 3.2.5 (Poles of W_5)**.** We illustrate Proposition 3.2.4 in the case $n = 5$. In particular, we demonstrate how to show that all poles are indeed simple. To this end, we start with the recursion:

$$\begin{aligned}(s+6)^4W_5(s+6)-(35(s+5)^4+42(s+5)^2+3)W_5(s+4)\\ +(s+4)^2(259(s+4)^2+104)W_5(s+2)=225(s+4)^2(s+2)^2W_5(s).\end{aligned}$$

From here,

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

which shows that the first pole is indeed simple as is also guaranteed by Proposition 3.2.4b. Similarly,

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

showing that the second pole is simple as well. It follows from Proposition 3.2.4c that all poles of W_5 are simple. More specifically, let $r_5(k) := \mathrm{Res}_{(-2k)}(W_5)$. With initial values $r_5(0) = 0, r_5(1)$ and $r_5(2)$, we derive that

$$\begin{aligned} r_5(k+3) &= \frac{k^4 r_5(k) - (5 + 28\,k + 63\,k^2 + 70\,k^3 + 35\,k^4)\, r_5(k+1)}{225(k+1)^2(k+2)^2} \\ &\quad + \frac{(285 + 518\,k + 259\,k^2)\, r_5(k+2)}{225(k+2)^2}. \end{aligned}$$

$\diamondsuit$

3.2.2 Meijer G-function representations

The *Meijer G-function* was introduced in 1936 by the Dutch mathematician Cornelis Simon Meijer (1904-1974). It is defined, for parameter vectors $\mathbf{a}$ and $\mathbf{b}$ [AAR99], by

$$\begin{aligned} G^{m,n}_{p,q}\left(\begin{matrix}\mathbf{a}\\ \mathbf{b}\end{matrix}\,\middle|\, x\right) &= G^{m,n}_{p,q}\left(\begin{matrix}a_1,\ldots,a_p\\ b_1,\ldots,b_q\end{matrix}\,\middle|\, x\right) \\ &= \frac{1}{2\pi i}\int_L \frac{\prod_{k=1}^m \Gamma(b_k - t)\prod_{k=1}^n \Gamma(1 - a_k + t)}{\prod_{k=m+1}^q \Gamma(1 - b_k + t)\prod_{k=n+1}^p \Gamma(a_k - t)}\, x^t \,\mathrm{d}t. \end{aligned} \tag{3.20}$$

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 $|x| > 1$. Moreover $G^{p,q}_{m,n}$ is analytic in each parameter; in consequence so are the compositions arising below.

Our main tool below is the following special case of Parseval's formula giving the Mellin transform of a product.

Theorem 3.2.6. *Let $G(s)$ and $H(s)$ be the Mellin transforms of $g(x)$ and $h(x)$ respectively. Then*

$$\int_0^\infty x^{s-1} g(x)h(x)\,\mathrm{d}x = \frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty} G(z)H(s-z)\,\mathrm{d}z \tag{3.21}$$

for any real number δ in the common region of analyticity.

This leads to:

Theorem 3.2.7 (Meijer form for W_3)**.** *For all complex s*

$$W_3(s) = \frac{\Gamma(1+s/2)}{\Gamma(1/2)\Gamma(-s/2)} G_{3,3}^{2,1}\left(\begin{matrix} 1,1,1 \\ 1/2,-s/2,-s/2 \end{matrix}\middle| \frac{1}{4}\right). \tag{3.22}$$

Proof. We apply Theorem 3.2.6 to $J_0^3 = J_0^2 \cdot J_0$ for s in a vertical strip. Using Example 3.2.2 we then obtain

$$\begin{aligned}
\int_0^\infty x^{s-1} J_0^3(x)\,\mathrm{d}x &= \frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty} \frac{2^{s-z-2}}{\Gamma(1/2)} \frac{\Gamma(z/2)\Gamma(1/2-z/2)}{\Gamma(1-z/2)^2} \frac{\Gamma(s/2-z/2)}{\Gamma(1-s/2+z/2)}\,\mathrm{d}z \\
&= \frac{2^s}{2\Gamma(1/2)} \frac{1}{2\pi i}\int_{\delta/2-i\infty}^{\delta/2+i\infty} 4^{-t} \frac{\Gamma(t)\Gamma(1/2-t)\Gamma(s/2-t)}{\Gamma(1-t)^2\Gamma(1-s/2+t)}\,\mathrm{d}t \\
&= \frac{2^s}{2\Gamma(1/2)} G_{3,3}^{2,1}\left(\begin{matrix} 1,1,1 \\ 1/2,s/2,s/2 \end{matrix}\middle| \frac{1}{4}\right)
\end{aligned}$$

where $0 < \delta < 1$. The claim follows from (3.17) by analytic continuation. □

Similarly we obtain:

Theorem 3.2.8 (Meijer form for W_4)**.** *For all complex s with* $\mathrm{Re}\, s > -2$

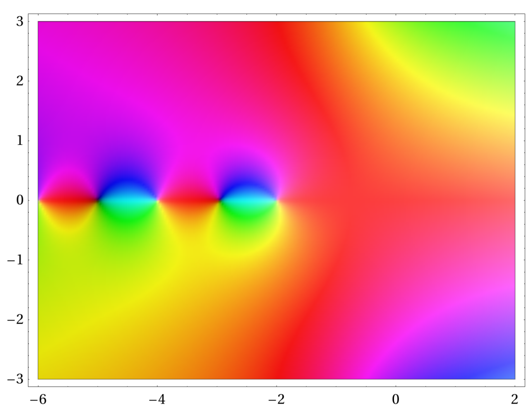
$$W_4(s) = \frac{2^s}{\pi} \frac{\Gamma(1+s/2)}{\Gamma(-s/2)} G_{4,4}^{2,2}\left(\begin{matrix} 1,(1-s)/2,1,1 \\ 1/2,-s/2,-s/2,-s/2 \end{matrix}\middle| 1\right). \tag{3.23}$$

Proof. We now apply Theorem 3.2.6 to $J_0^4 = J_0^2 \cdot J_0^2$, again for s in a vertical strip. Using once more Example 3.2.2, we obtain

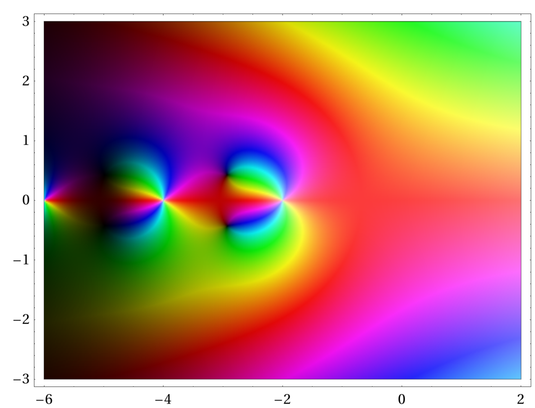
$$\begin{aligned}\int_0^\infty x^{s-1} J_0^4(x)\,\mathrm{d}x &= \frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty} \frac{1}{4\pi}\frac{\Gamma(z/2)\Gamma(1/2-z/2)}{\Gamma(1-z/2)^2}\frac{\Gamma(s/2-z/2)\Gamma(1/2-s/2+z/2)}{\Gamma(1-s/2+z/2)^2}\,\mathrm{d}z\\ &= \frac{1}{2\pi} G^{2,2}_{4,4}\left(\begin{matrix}1,(1+s)/2,1,1\\ 1/2,s/2,s/2,s/2\end{matrix}\middle|1\right)\end{aligned}$$

where $0<\delta<1$. The claim again follows from (3.17). $\square$

We illustrate with graphs of W_3, W_4 in the complex plane in Figure 3.2. Note the poles, which are white, and zeros, which are black (other complex numbers are assigned a (non-unique) color depending on argument and modulus in such a way that the order of poles and zeros is visible). These graphs were produced employing the Meijer forms in their hypergeometric form as presented in the next section. In the case $n=4$, the functional equation is employed for s with $\operatorname{Re} s \leqslant -2$.



(a) W_3



(b) W_4

Figure 3.2: W_3 via (3.22) and W_4 via (3.23) in the complex plane.

3.2.3 Hypergeometric representations

By Slater's theorem [Mar83, p. 57], the Meijer G-function representations for $W_3(s)$ and $W_4(s)$ given in Theorems 3.2.7 and 3.2.8 can be expanded in terms of generalized hypergeometric functions.

Corollary 3.2.9 (Hypergeometric forms)**.** *For s not an odd integer, we have*

$$W_3(s) = \frac{1}{2^{2s+1}} \tan\left(\frac{\pi s}{2}\right) \binom{s}{\frac{s-1}{2}}^2 {}_3F_2\left({\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{s+3}{2}, \frac{s+3}{2}} \middle| \frac{1}{4} \right) + \binom{s}{\frac{s}{2}} {}_3F_2\left({-\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \atop 1, -\frac{s-1}{2}} \middle| \frac{1}{4} \right), \tag{3.24}$$

and, if also $\operatorname{Re} s > -2$*, we have*

$$W_4(s) = \frac{1}{2^{2s}} \tan\left(\frac{\pi s}{2}\right) \binom{s}{\frac{s-1}{2}}^3 {}_4F_3\left({\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{s}{2}+1 \atop \frac{s+3}{2}, \frac{s+3}{2}, \frac{s+3}{2}} \middle| 1 \right) + \binom{s}{\frac{s}{2}} {}_4F_3\left({\frac{1}{2}, -\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \atop 1, 1, -\frac{s-1}{2}} \middle| 1 \right). \tag{3.25}$$

These lovely analytic continuations of W_3 and W_4, first found in [Cra09], can also be obtained by symbolic integration of (3.11) in *Mathematica*.

Example 3.2.10. From (3.24) and taking the limit using L'Hôpital's rule, we have

$$W_3(-1) = \frac{16}{\pi^3} \mathrm{K}^2\left(\frac{\sqrt{3}-1}{2\sqrt{2}}\right) \log 2 + \frac{3}{\pi} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^3}{4^{4n}} \sum_{k=1}^{2n} \frac{(-1)^k}{k}. \tag{3.26}$$

In conjunction with (3.7) we obtain

$$\sum_{n=0}^{\infty} \binom{2n}{n}^3 \frac{\sum_{k=1}^{2n} \frac{(-1)^k}{k}}{4^{4n}} = \left(\frac{2}{\sqrt{3}\pi} - \frac{16}{3\pi^2} \log 2\right) \mathrm{K}^2\left(\frac{\sqrt{3}-1}{2\sqrt{2}}\right). \tag{3.27}$$

For comparison, (3.25) produces

$$W_4(-1) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4}{4^{4n}} \sum_{k=2n+1}^{\infty} \frac{(-1)^{k+1}}{k}.$$

◊

We see that while Corollary 3.2.9 makes it easy to analyse the poles, the provably removable singularities at odd integers are much harder to resolve explicitly [Cra09]. For $W_4(-1)$ we proceed as follows:

Theorem 3.2.11 (Hypergeometric form for $W_4(-1)$)**.**

$$W_4(-1) = \frac{\pi}{4}\,{}_7F_6\left(\begin{matrix}\frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{1}{4}, 1, 1, 1, 1, 1\end{matrix}\middle| 1\right). \tag{3.28}$$

Proof. Using Theorem 3.2.8 we write

$$W_4(-1) = \frac{1}{2\pi} G_{4,4}^{2,2}\left(\begin{matrix}1, 1, 1, 1 \\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\end{matrix}\middle| 1\right).$$

Using the definition (3.20) of the Meijer G-function as a contour-integral, we see that the corresponding integrand is

$$\frac{\Gamma(\frac{1}{2}-t)^2\Gamma(t)^2}{\Gamma(\frac{1}{2}+t)^2\Gamma(1-t)^2}x^t = \frac{\Gamma(\frac{1}{2}-t)^2\Gamma(t)^4}{\Gamma(\frac{1}{2}+t)^2} \cdot \frac{\sin^2(\pi t)}{\pi^2}x^t, \tag{3.29}$$

where we have used $\Gamma(t)\Gamma(1-t) = \frac{\pi}{\sin(\pi t)}$. We choose the contour of integration to enclose the poles of $\Gamma(\frac{1}{2}-t)$. Note then that the presence of $\sin^2(\pi t)$ does not interfere with the contour or the residues (for $\sin^2(\pi t) = 1$ at half integers). Hence we may ignore $\sin^2(\pi t)$ in the integrand altogether. Then the right-hand side of (3.29) is the integrand of another Meijer G-function; thus we have shown that

$$G_{4,4}^{2,2}\left(\begin{matrix}1, 1, 1, 1 \\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\end{matrix}\middle| 1\right) = \frac{1}{\pi^2} G_{4,4}^{2,4}\left(\begin{matrix}1, 1, 1, 1 \\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\end{matrix}\middle| 1\right). \tag{3.30}$$

The same argument shows that the factor of $\frac{1}{\pi^2}$ applies to all $W_4(s)$ when we change from $G_{4,4}^{2,2}$ to $G_{4,4}^{2,4}$.

Now, using the transformation

$$x^\alpha G^{m,n}_{p,q}\left(\begin{matrix}\mathbf{a}\\ \mathbf{b}\end{matrix}\middle| x\right) = G^{m,n}_{p,q}\left(\begin{matrix}\mathbf{a}+\alpha\\ \mathbf{b}+\alpha\end{matrix}\middle| x\right) \tag{3.31}$$

we deduce that

$$W_4(-1) = \frac{1}{2\pi^3} G^{2,4}_{4,4}\left(\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ 0,0,0,0\end{matrix}\middle| 1\right).$$

Finally, we appeal to Bailey's identity [Bai32, Formula (3.4)]:

$$\begin{aligned}
&{}_7F_6\left(\begin{matrix}a, 1+\frac{a}{2}, b, c, d, e, f\\ \frac{a}{2}, 1+a-b, 1+a-c, 1+a-d, 1+a-e, 1+a-f\end{matrix}\middle| 1\right)\\
&= \frac{\Gamma(1+a-b)\Gamma(1+a-c)\Gamma(1+a-d)\Gamma(1+a-e)\Gamma(1+a-f)}{\Gamma(1+a)\Gamma(b)\Gamma(c)\Gamma(d)\Gamma(1+a-b-c)\Gamma(1+a-b-d)\Gamma(1+a-c-d)\Gamma(1+a-e-f)}\\
&\quad\times G^{2,4}_{4,4}\left(\begin{matrix}e+f-a, 1-b, 1-c, 1-d\\ 0, 1+a-b-c-d, e-a, f-a\end{matrix}\middle| 1\right).
\end{aligned} \tag{3.32}$$

The claim follows upon setting all parameters to 1/2. □

An attempt to analogously apply Bailey's identity for $W_4(1)$ fails, since its Meijer G representation as obtained from Theorem 3.2.8 does not meet the precise form required in the formula. Nevertheless, a combination of Nesterenko's theorem ([Nes03]) and Zudilin's theorem ([Zud02]) gives the following result:

Theorem 3.2.12 (Hypergeometric form for $W_4(1)$)**.**

$$W_4(1) = \frac{3\pi}{4}\,{}_7F_6\left(\begin{matrix}\frac{7}{4},\frac{3}{2},\frac{3}{2},\frac{3}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{3}{4},2,2,2,1,1\end{matrix}\middle| 1\right) - \frac{3\pi}{8}\,{}_7F_6\left(\begin{matrix}\frac{7}{4},\frac{3}{2},\frac{3}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{3}{4},2,2,2,2,1\end{matrix}\middle| 1\right). \tag{3.33}$$

Proof. We first prove a result that will allow us to use Nesterenko's theorem, which converts the Meijer G form of $W_4(1)$ to a triple integral. We need the following identities which can be readily verified:

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(z^{-b_1} G_{4,4}^{2,2}\left(\begin{matrix} a_1, a_2, a_3, a_4 \\ b_1, b_2, b_3, b_4 \end{matrix} \middle| z\right)\right) = -z^{-1-b_1} G_{4,4}^{2,2}\left(\begin{matrix} a_1, a_2, a_3, a_4 \\ b_1+1, b_2, b_3, b_4 \end{matrix} \middle| z\right) \tag{3.34}$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\left(z^{1-a_1} G_{4,4}^{2,2}\left(\begin{matrix} a_1, a_2, a_3, a_4 \\ b_1, b_2, b_3, b_4 \end{matrix} \middle| z\right)\right) = z^{-a_1} G_{4,4}^{2,2}\left(\begin{matrix} a_1-1, a_2, a_3, a_4 \\ b_1, b_2, b_3, b_4 \end{matrix} \middle| z\right) \tag{3.35}$$

Let $a(z) := G_{4,4}^{2,2}\left(\begin{smallmatrix} 0,1,1,1 \\ -\frac{1}{2},\frac{1}{2},-\frac{1}{2},-\frac{1}{2} \end{smallmatrix} \middle| z\right)$. Note that $a(1) = -2\pi W_4(1)$ by Theorem 3.2.8. Applying (3.34) to $a(z)$ and using the product rule, we get $\frac{1}{2}a(1) + a'(1) = c_1$, where $c_1 := -G_{4,4}^{2,2}\left(\begin{smallmatrix} 0,1,1,1 \\ \frac{1}{2},\frac{1}{2},-\frac{1}{2},-\frac{1}{2} \end{smallmatrix} \middle| 1\right)$. Applying (3.35) and (3.31) to $a(z)$, we obtain $a'(1) = b_1$ where $b_1 := G_{4,4}^{2,2}\left(\begin{smallmatrix} -\frac{1}{2},-\frac{1}{2},\frac{1}{2},\frac{1}{2} \\ 0,-1,-1,-1 \end{smallmatrix} \middle| 1\right)$. Appealing to equation (3.65), we see that $b_1 = -c_1$. Hence $a(1) = 4c_1$. Converting c_1 to a $G_{4,4}^{2,4}$ as in (3.30), which finally satisfies the conditions of Nesterenko's theorem, we obtain:

$$W_4(1) = \frac{4}{\pi^3}\int_0^1\int_0^1\int_0^1 \sqrt{\frac{x(1-y)(1-z)}{(1-x)yz(1-x(1-yz))}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z.$$

We now make a change of variable $z' = 1-z$. Writing

$$(z')^{\frac{1}{2}} = (z')^{-\frac{1}{2}}(1-(1-z')) = (z')^{-\frac{1}{2}} - (z')^{-\frac{1}{2}}(1-z')$$

splits the previous triple integral into two terms. Each term satisfies Zudilin's theorem and so can be written as a ${}_7F_6$. We thence obtain the result as claimed. □

The following alternative relation was first predicted by the *integer relation algorithm* PSLQ in a computational hunt for results similar to that in Theorem 3.2.11:

Theorem 3.2.13 (Alternative hypergeometric form for $W_4(1)$)**.**

$$W_4(1) = \frac{9\pi}{4}\,{}_7F_6\left(\begin{matrix} \frac{7}{4},\frac{3}{2},\frac{3}{2},\frac{3}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2} \\ \frac{3}{4},2,2,2,1,1 \end{matrix} \middle| 1\right) - 2\pi\,{}_7F_6\left(\begin{matrix} \frac{5}{4},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2} \\ \frac{1}{4},1,1,1,1,1 \end{matrix} \middle| 1\right). \tag{3.36}$$

Proof. For notational convenience, let

$$\begin{aligned} A &:= \frac{3\pi^4}{128}\, {}_7F_6\left(\left.{\frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{3}{4}, 2, 2, 2, 1, 1}\right| 1\right), \\ B &:= \frac{3\pi^4}{256}\, {}_7F_6\left(\left.{\frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{3}{4}, 2, 2, 2, 2, 1}\right| 1\right), \\ C &:= \frac{\pi^4}{16}\, {}_7F_6\left(\left.{\frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{1}{4}, 1, 1, 1, 1, 1}\right| 1\right). \end{aligned}$$

By (3.33), $W_4(1) = (32/\pi^3)(A - B)$, and the truth of (3.36) is equivalent to the evaluation $W_4(1) = (32/\pi^3)(3A - C)$. Thus, we only need to show $2A + B - C = 0$.

The triple integral for A encountered in the application of Zudilin's theorem is

$$A = \frac{1}{8}\int_0^1\int_0^1\int_0^1 \sqrt{\frac{x(1-y)}{(1-x)yz(1-z)(1-x(1-yz))}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z,$$

and can be reduced to a one dimensional integral:

$$A = A_1 := \int_0^1 \frac{(K'(k) - E'(k))^2}{1-k^2}\,\mathrm{d}k,$$

Here, as usual, $K'(k) := K\left(\sqrt{1-k^2}\right)$ and $E'(k) := E(\sqrt{1-k^2})$.

Happily, we may apply a non-trivial action on the exponents of x, y, z and leave the value of the integral unchanged (see [Zud04], remark after lemma 8). We obtain:

$$\begin{aligned} A &= \frac{1}{8}\int_0^1\int_0^1\int_0^1 \sqrt{\frac{1-x(1-yz)}{xyz(1-x)(1-y)(1-z)}}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \\ &= A_2 := \int_0^1 K'(k)E'(k)\,\mathrm{d}k. \end{aligned}$$

The like integral for B can also be reduced to a one dimensional integral,

$$B = B_2 := \int_0^1 k^2 K'(k)^2\,\mathrm{d}k.$$

But B also satisfies the conditions of Bailey's identity and Nesterenko's theorem, from which we are able to produce an alternative triple integral, and reduce it to:

$$B = B_1 := \int_0^1 (K'(k) - E'(k)) \left(E'(k) - k^2 K'(k)\right) \frac{\mathrm{d}k}{1-k^2}.$$

As for C, equation (3.57) details its evaluation, which we also record here:

$$C = \int_0^1 K'(k)^2 \,\mathrm{d}k.$$

Now $2A+B-C = A_1+A_2+B_1-C = 0$, because the integrand of the later expression is zero. $\square$

Note that the theorem gives the identity

$$2\int_0^1 K'(k)E'(k)\,\mathrm{d}k = \int_0^1 (1-k^2)K'(k)^2\,\mathrm{d}k, \tag{3.37}$$

among others. An ensuing systematic study of the moments of products of elliptic integrals may be found in [Wan12].

Remark 3.2.14. Note that each of the ${}_7F_6$'s involved in Theorems 3.2.11, 3.2.12 and 3.2.13 can also be easily written as a sum of two ${}_6F_5$'s.

Also note that the first ${}_7F_6$ term in Theorem 3.2.13 satisfies the conditions of Bailey's identity (3.32) (with $a = e = f = \frac{3}{2}, b = c = d = \frac{1}{2}$):

$${}_7F_6\left(\left.\begin{matrix}\frac{7}{4},\frac{3}{2},\frac{3}{2},\frac{3}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{3}{4},2,2,2,1,1\end{matrix}\right|1\right) = -\frac{16}{3\pi^4}G^{2,4}_{4,4}\left(\left.\begin{matrix}\frac{3}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ 1,0,0,0\end{matrix}\right|1\right). \tag{3.38}$$

We can thence convert the right-hand side to a Meijer G form. On the other hand,

$$W_4(1) = -\frac{1}{2\pi^3}G^{2,4}_{4,4}\left(\left.\begin{matrix}0,1,1,1\\ \frac{1}{2},-\frac{1}{2},-\frac{1}{2},-\frac{1}{2}\end{matrix}\right|1\right).$$

We thus obtain the non-trivial identity:

$$G_{4,4}^{2,4}\left(\begin{matrix}\frac{1}{2},\frac{3}{2},\frac{3}{2},\frac{3}{2}\\1,0,0,0\end{matrix}\middle|1\right) = 24\,G_{4,4}^{2,4}\left(\begin{matrix}\frac{3}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\1,0,0,0\end{matrix}\middle|1\right) + 8\,G_{4,4}^{2,4}\left(\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2}\\0,0,0,0\end{matrix}\middle|1\right). \tag{3.39}$$

♢

Corollary 3.2.15 (Elliptic integral representation for $W_4(1)$)**.** *We have*

$$W_4(1) = \frac{16}{\pi^3}\int_0^1 (1-3k^2)K'(k)^2\,\mathrm{d}k. \tag{3.40}$$

Proof. The conclusion of Theorem 3.2.13 implies $(\pi^3/16)\,W_4(1) = C - 3B = C - 3B_2$. □

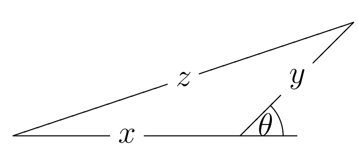
3.3 Probabilistically inspired representations

In this section, we build on the probabilistic approach taken in Section 6 of [BNSW11]. We may profitably view a $(m+n)$-step walk as a composition of an m-step and n-step walk for $m, n \geqslant 1$. Different decompositions make different structures apparent.

We express the distance z of an $(n+m)$-step walk conditioned on a given distance x of the first n steps as well as the distance y of the remaining m steps. Then, by the cosine rule,

$$z^2 = x^2 + y^2 + 2xy\cos(\theta),$$

where θ is the outside angle of the triangle with sides of lengths x, y, and z:



It follows that for $s>0$, the s-th moment of an $(n+m)$-step walk conditioned on the distance x of the first n steps and the distance y of the remaining m steps is

$$g_s(x,y) := \frac{1}{\pi}\int_0^\pi z^s \,\mathrm{d}\theta = |x-y|^s \,{}_2F_1\left(\left.{\frac{1}{2}, -\frac{s}{2} \atop 1}\right| -\frac{4xy}{(x-y)^2}\right). \tag{3.41}$$

Here we appealed to symmetry to restrict the angle to $\theta \in [0,\pi)$. We then evaluated the integral in hypergeometric form which, for instance, can be done with the help of *Mathematica* or *Maple*.

Remark 3.3.1 (Alternate forms for g_s)**.** Using Kummer's quadratic transformation [AAR99], we obtain

$$g_s(x,y) = \operatorname{Re}\, y^s \,{}_2F_1\left(\left.{-\frac{s}{2}, -\frac{s}{2} \atop 1}\right| \frac{x^2}{y^2}\right) \tag{3.42}$$

for general positive x,y. This provides an analytic continuation of $s \mapsto g_s(x,y)$. In particular, we have

$$g_{-1}(x,y) = \frac{2}{\pi}\operatorname{Re}\frac{1}{y}\,K\left(\frac{x}{y}\right) \tag{3.43}$$

and, with E the complete elliptic integral of the second kind, we have

$$g_1(x,y) = \frac{2}{\pi}\operatorname{Re}\, y\left\{2E\left(\frac{x}{y}\right) - \left(1-\frac{x^2}{y^2}\right)K\left(\frac{x}{y}\right)\right\}. \tag{3.44}$$

This later form has various re-expressions. ♢

Denote by $p_n(x)$ the density of the distance x for an n-step walk. Since $W_{n+m}(s)$ is the s-th moment of the distance of an $(n+m)$-step walk, we obtain

$$W_{n+m}(s) = \int_0^n\int_0^m g_s(x,y)\,p_n(x)p_m(y)\,\mathrm{d}y\,\mathrm{d}x, \tag{3.45}$$

for $s \geqslant 0$. Since for the 1-step walk we have $p_1(x) = \delta_1(x)$, this generalizes the corresponding formula given for $W_{n+1}(s)$ in [BNSW11].

In (3.45), if $n = 0$, then we may take $p_0(x) = \delta_0(x)$, and regard the limits of integration as from $-\epsilon$ and $+\epsilon$, $\epsilon \to 0$. Then $g_s = y^s$ as the hypergeometric collapses to 1, and we recover the basic form

$$W_m(s) = \int_0^m y^s p_m(y)\,\mathrm{d}y. \tag{3.46}$$

It is also easily shown that the probability density for a 2-step walk is given by

$$p_2(x) = \frac{2}{\pi\sqrt{4-x^2}}$$

for $0 \leqslant x \leqslant 2$ and 0 otherwise.

The density $p_3(x)$ for $0 \leqslant x \leqslant 3$ can be expressed by

$$p_3(x) = \mathrm{Re}\left(\frac{\sqrt{x}}{\pi^2}\,K\left(\sqrt{\frac{(x+1)^3(3-x)}{16x}}\right)\right), \tag{3.47}$$

see, e.g., [Pea06]. To make (3.47) more accessible we need the following cubic identity.

Proposition 3.3.2. *For all* $0 \leqslant x \leqslant 1$ *we have*

$$K\left(\sqrt{\frac{16x^3}{(3-x)^3(1+x)}}\right) = \frac{3-x}{3+3x}\,K\left(\sqrt{\frac{16x}{(3-x)(1+x)^3}}\right).$$

Proof. Both sides satisfy the differential equation

$$4x^2(x+3)^2 f(x) + (x-3)(x+1)^2((x^3-9x^2-9x+9)f'(x) + x(x^3-x^2-9x+9)f''(x)) = 0,$$

and both of their function values and derivative values agree at the origin. $\square$

Applying Jacobi's imaginary transform [BB98, p. 73], $\mathrm{Re}\,K(x) = \frac{1}{x}K\left(\frac{1}{x}\right)$, for

$x > 1$ to express $p_3(x)$ as a real function over $[0,1]$ and $[1,3]$, leads to

$$W_3(-1) = \int_0^3 \frac{p_3(x)}{x}\,\mathrm{d}x = \frac{4}{\pi^2}\int_0^1 \frac{K\left(\sqrt{\frac{16x}{(3-x)(1+x)^3}}\right)}{\sqrt{(3-x)(1+x)^3}}\,\mathrm{d}x + \frac{1}{\pi^2}\int_1^3 \frac{K\left(\sqrt{\frac{(3-x)(1+x)^3}{16x}}\right)}{\sqrt{x}}\,\mathrm{d}x.$$

The change of variables $x \to \frac{3-t}{1+t}$ in the last integral transforms it into the second last integral. Therefore,

$$W_3(-1) = 2\int_0^1 \frac{p_3(x)}{x}\,\mathrm{d}x. \tag{3.48}$$

To make sense of this more abstractly, let

$$\sigma(x) = \frac{3-x}{1+x}, \qquad \lambda(x) = \frac{(1+x)^3(3-x)}{16x}.$$

Then for $0 < x < 3$ we have $\sigma^2(x) = x$ and $\lambda(x)\lambda(\sigma(x)) = 1$. In consequence σ is an involution that sends $[0,1]$ to $[1,3]$ and

$$p_3(x) = \frac{4x}{(3-x)(x+1)}\,p_3(\sigma(x)). \tag{3.49}$$

Example 3.3.3 (Series for p_3 and $W_3(-1)$)**.** We know that

$$W_3(2k) = \sum_{j=0}^{k} \binom{k}{j}^2 \binom{2j}{j}$$

is the sum of squares of trinomials (see (3.8) and [BNSW11]). Using Proposition 3.3.2, we may now apply equation (184) in [BBBG08, Section 5.10] to obtain

$$p_3(x) = \frac{2x}{\pi\sqrt{3}} \sum_{k=0}^{\infty} W_3(2k)\left(\frac{x}{3}\right)^{2k}, \tag{3.50}$$

with radius of convergence 1. From (3.50) and (3.48) we deduce that

$$W_3(-1) = \frac{4}{\pi\sqrt{3}} \sum_{k=0}^{\infty} \frac{W_3(2k)}{9^k(2k+1)}$$

as a type of reflection formula. $\lozenge$

We can use (3.10) to deduce for all $n \geqslant 4$ that

$$p_n(\alpha) = \alpha \int_0^\infty J_0(t)^n J_0(\alpha t) t \, \mathrm{d}t. \tag{3.51}$$

Alternatively, setting $\phi_n(r) := p_n(r)/(2\pi r)$, we have that for $n \geqslant 2$ ([Hug95])

$$\phi_n(r) = \frac{1}{2\pi} \int_0^{2\pi} \phi_{n-1}\left(\sqrt{r^2+1-2r\cos t}\right) \mathrm{d}t. \tag{3.52}$$

The densities p_3 and p_4 are shown in Figure 3.3. Note that p_3 has a singularity at 1 as follows from (3.47). We remark that the derivative of p_4 has singularities at 0 and 4. We also record that $p_4^-(2) \approx .144687$ while $p_4^+(2) = -\infty$. This can be proven by using the large-order asymptotic expansion for J_ν to estimate $p_4'(s)$ for s near 2 as a combination of Fresnel integrals.

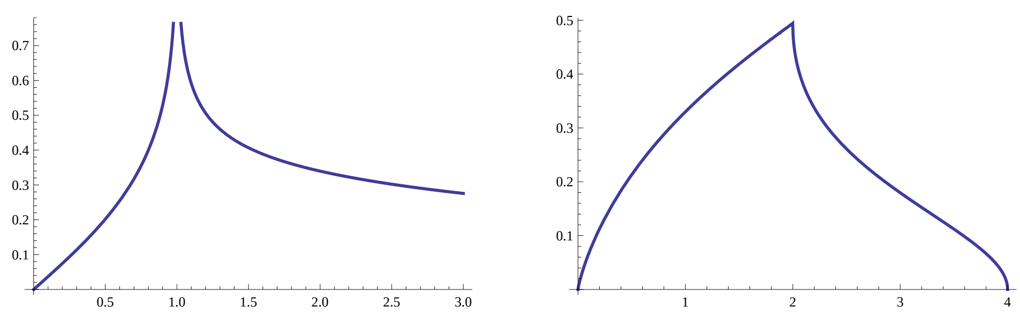


Figure 3.3: The densities p_3 (L) and p_4 (R).

Example 3.3.4 (Poles of W_3)**.** From here we may efficiently recover the explicit form for the residues of W_3 given in Proposition 3.2.4a. Fix integers $N > 2k > 0$ and

$0 < \alpha < 1$. Use the series $p_3(x) = \sum_{j\geqslant 0} a_j x^{2j+1}$ in (3.50) to write

$$\begin{aligned} W_3(s) - \int_\alpha^3 p_3(x)x^s \,\mathrm{d}x - \int_0^\alpha \sum_{j=N}^{\infty} a_j x^{2j+1+s} \,\mathrm{d}x &= \int_0^\alpha \sum_{j=0}^{N-1} a_j x^{2j+1+s} \,\mathrm{d}x \\ &= \sum_{j=1}^{N} a_{j-1} \frac{\alpha^{2j+s}}{2j+s}, \end{aligned} \tag{3.53}$$

and observe that both sides are holomorphic and so (3.53) holds in a neighborhood of $s = -2k$. Since only the first term on the left has a pole at $-2k$ we may deduce that $\mathrm{Res}_{(-2k)}(W_3) = a_{k-1}$. Equivalently,

$$\mathrm{Res}_{(-2k-2)}(W_3) = \frac{2}{\pi\sqrt{3}} \frac{W_3(2k)}{3^{2k}},$$

which exposes an elegant reflection property. ♢

Remark 3.3.5 (W_5)**.** Using (3.45) we may express $W_5(s)$ and $W_6(s)$ as double integrals, for example,

$$W_5(-1) = \frac{4}{\pi^4} \int_0^3 \int_0^2 \frac{\sqrt{x}}{y\sqrt{4-y^2}} \,\mathrm{Re}\left(K\left(\frac{x}{y}\right)\right) \mathrm{Re}\left(K\left(\sqrt{\frac{(x+1)^3(3-x)}{16x}}\right)\right) \mathrm{d}y \,\mathrm{d}x.$$

We also have an expression based on taking two 2-step walks and a 1-step walk:

$$\begin{aligned} W_5(-1) &= \frac{8}{\pi^4} \int_0^2 \int_0^2 \int_0^\pi \frac{\mathrm{Re}\ K(\sqrt{x^2+y^2+2xy\cos z})}{\sqrt{(4-x^2)(4-y^2)}} \,\mathrm{d}z \,\mathrm{d}x \,\mathrm{d}y \\ &= \frac{8}{\pi^4} \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} \int_0^\pi \mathrm{Re}\ K\left(2\sqrt{\sin^2 a + \sin^2 b + 2\sin a \sin b \cos c}\right) \mathrm{d}c \,\mathrm{d}a \,\mathrm{d}b, \end{aligned}$$

but we have been unable to make further progress with these forms. ♢

3.3.1 Elliptic integral representations

From (3.45), we derive

$$\begin{aligned} W_4(s) &= \frac{2^{s+2}}{\pi^2}\int_0^1\int_0^1 \frac{g_s(x,y)}{\sqrt{(1-x^2)(1-y^2)}}\,\mathrm{d}x\,\mathrm{d}y \\ &= \frac{2^{s+2}}{\pi^2}\int_0^{\pi/2}\int_0^{\pi/2} g_s(\sin u, \sin v)\,\mathrm{d}u\,\mathrm{d}v. \end{aligned}$$

where $s > -2$. In particular, for $s = -1$, again using Jacobi's imaginary transformation, we have:

$$\begin{aligned} W_4(-1) &= \frac{4}{\pi^3}\,\mathrm{Re}\int_0^1\int_0^1 \frac{K(x/y)}{y\sqrt{(1-x^2)(1-y^2)}}\,\mathrm{d}x\,\mathrm{d}y \qquad (3.54) \\ &= \frac{8}{\pi^3}\int_0^1\int_0^1 \frac{K(t)}{\sqrt{(1-t^2y^2)(1-y^2)}}\,\mathrm{d}y\,\mathrm{d}t \\ &= \frac{8}{\pi^3}\int_0^1 K^2(k)\,\mathrm{d}k. \qquad (3.55) \end{aligned}$$

The corresponding integral at $s = 1$ is

$$W_4(1) = \frac{32}{\pi^3}\int_0^1 \frac{(k+1)(K(k)-E(k))}{k^2}\; E\left(\frac{2\sqrt{k}}{k+1}\right)\mathrm{d}k.$$

Starting with Nesterenko's theorem [Nes03] we have the following:

$$W_4(-1) = \frac{1}{2\pi^3}\int_{[0,1]^3} \frac{\mathrm{d}x\mathrm{d}y\mathrm{d}z}{\sqrt{xyz(1-x)(1-y)(1-z)(1-x(1-yz))}}. \qquad (3.56)$$

(Such integrals are related to Beukers' integrals, which were used in the elementary derivation of the irrationality of $\zeta(3)$.) Upon computing the dx integral, followed by the change of variable $k^2 = yz$, we have:

$$W_4(-1) = \frac{1}{\pi^3}\int_0^1\int_0^1 \frac{K(\sqrt{1-yz})}{\sqrt{yz(1-y)(1-z)}}\,\mathrm{d}y\,\mathrm{d}z \tag{3.57}$$

$$= \frac{2}{\pi^3}\int_0^1\int_{k^2}^1 \frac{K(\sqrt{1-k^2})}{\sqrt{y(1-y)(y-k^2)}}\,\mathrm{d}y\,\mathrm{d}k$$

$$= \frac{4}{\pi^3}\int_0^1 K'(k)^2\,\mathrm{d}k. \tag{3.58}$$

Compare this with the corresponding (3.54). In particular, appealing to Theorem 3.2.11 we derive the closed forms:

$$2\int_0^1 K(k)^2\,\mathrm{d}k = \int_0^1 K'(k)^2\,\mathrm{d}k = \left(\frac{\pi}{2}\right)^4 {}_7F_6\left(\left.{\frac{5}{4},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2} \atop \frac{1}{4},1,1,1,1,1}\right|1\right). \tag{3.59}$$

Recalling Corollary 3.2.15 and equation (3.37) we also deduce that

$$W_4(1) = \frac{96}{\pi^3}\int_0^1 E'(k)K'(k)\,\mathrm{d}k - 8\,W_4(-1). \tag{3.60}$$

If we make a trigonometric change of variables in (3.57), we obtain

$$W_4(-1) = \frac{4}{\pi^3}\int_0^{\pi/2}\int_0^{\pi/2} K\left(\sqrt{1-\sin^2 x\sin^2 y}\right)\mathrm{d}x\,\mathrm{d}y. \tag{3.61}$$

We may rewrite the integrand as a sum, and then interchange integration and summation to arrive at a slowly convergent representation of the same general form as in Conjecture 3.1.1:

$$W_4(-1) = \frac{1}{2}\sum_{n=0}^{\infty}\binom{-1/2}{n}^2 {}_3F_2\left(\left.{\frac{1}{2},\frac{1}{2},-n \atop 1,1}\right|1\right). \tag{3.62}$$

Remark 3.3.6 (Relation to Watson integrals)**.** From the evaluation (3.7) we note that $W_3(-1)$ equals twice the second of three triple integrals considered by Watson in [Wat38]:

$$W_3(-1) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \frac{\mathrm{d}u\mathrm{d}v\mathrm{d}w}{3-\cos v\cos w-\cos w\cos u-\cos u\cos v}. \tag{3.63}$$

This is derived in [BBG04] and various related extensions are to be found in [BBBG08]. It is not clear how to generalize this to $W_4(-1)$.

Watson's second integral (3.63) also gives the alternative representation:

$$W_3(-1) = \pi^{-5/2} G_{3,3}^{3,2}\left(\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ 0,0,0\end{matrix}\middle|4\right). \tag{3.64}$$

The equivalence of this and the Meijer G representation coming from Theorem 3.2.7 can be established similarly to the proof of Theorem 3.2.11 upon using the Meijer G transformation

$$G_{p,q}^{m,n}\left(\begin{matrix}\mathbf{a}\\ \mathbf{b}\end{matrix}\middle|x\right) = G_{q,p}^{n,m}\left(\begin{matrix}1-\mathbf{b}\\ 1-\mathbf{a}\end{matrix}\middle|\frac{1}{x}\right). \tag{3.65}$$

$\diamondsuit$

Remark 3.3.7 (Probability of return to the unit disk)**.** By a simple geometric argument, there is a $\frac{1}{3}$ chance of returning to the unit disk in a 2-step walk. Similarly, for a 3-step walk, if the second step makes an angle θ with the first step, then the third step can only vary over a range of θ to return to the unit disk (it can be parallel to the first step, to the second step, or anywhere in between). Thus the probability of returning to the unit disk in three steps is

$$\frac{1}{4\pi^2}\int_{-\pi}^{\pi}|\theta|\,\mathrm{d}\theta = \frac{1}{4} = \int_0^1 p_3(x)\,\mathrm{d}x.$$

Appealing to (3.50) we deduce that

$$\sum_{k=0}^{\infty}\frac{W_3(2k)}{9^k(k+1)} = \frac{\sqrt{3}\pi}{4}.$$

In fact, as Kluyver showed [Klu06], the probability of an n-step walk ending in the unit disk is $1/(n+1)$. This is easily obtained by setting $\alpha = 1$ in (3.10). See also [Ber10] for a very short proof of this fact which is not based on a Bessel integral representation. $\Diamond$

3.4 Partial resolution of Conjecture 3.1.1

We may now investigate Conjecture 3.1.1 which is restated below for convenience.

Conjecture. For positive integers n and complex s,

$$W_{2n}(s) \stackrel{?[1]}{=} \sum_{j \geqslant 0} \binom{s/2}{j}^2 W_{2n-1}(s-2j). \tag{3.66}$$

We can resolve this conjecture modulo a conjectured technical estimate given in Conjecture 3.4.2. The proof outline below certainly explains Conjecture 3.1.1 by identifying the terms of the infinite sum as natural residues.

Proof. Using (3.17) we write W_{2n} as a Bessel integral

$$W_{2n}(-s) = 2^{1-s} \frac{\Gamma(1-s/2)}{\Gamma(s/2)} \int_0^\infty x^{s-1} J_0^{2n}(x) \, \mathrm{d}x.$$

Then we apply Theorem 3.2.6 to $J_0^{2n} = J_0^{2n-1} \cdot J_0$ for s in a vertical strip. Since, again by (3.17), we have

$$\int_0^\infty x^{s-1} J_0^{2n}(x) \, \mathrm{d}x = 2^{s-1} \frac{\Gamma(s/2)}{\Gamma(1-s/2)} W_n(-s)$$

we obtain

$$\begin{aligned} W_{2n}(-s) &= 2^{1-s}\frac{\Gamma(1-s/2)}{\Gamma(s/2)}\int_0^\infty x^{s-1}J_0^{2n-1}(x)\cdot J_0(x)\,\mathrm{d}x \\ &= \frac{\Gamma(1-s/2)}{\Gamma(s/2)}\frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty}\frac{1}{2}\frac{\Gamma(z/2)\Gamma(s/2-z/2)}{\Gamma(1-z/2)\Gamma(1-s/2+z/2)}W_{2n-1}(-z)\,\mathrm{d}z \end{aligned} \tag{3.67}$$

where $0<\delta<1$.

Observe that the integrand has poles at $z=s,s+2,s+4,\ldots$ coming from $\Gamma(s/2-z/2)$ as well as (irrelevant for current purposes) poles at $z=0,-2,-4,\ldots$ coming from $\Gamma(z/2)$. On the other hand, the term $W_{2n-1}(-z)$ has at most simple poles at $z=2,4,6,\ldots$ which are cancelled by the corresponding zeros of $\Gamma(1-z/2)$. This asserted pole structure of W_{2n-1} was shown in Example 3.2.5 for $n=3$ and may be shown analogously for each $n=4,5,\ldots$ based on Proposition 3.2.4. That this works generally is stated as Conjecture 3.4.1 below.

Next, we determine the residue of the integrand at $z=s+2j$. Since $\Gamma(s/2-z/2)$ has a residue of $-2(-1)^j/j!$ at $z=s+2j$, the residue of the integrand is

$$-\frac{(-1)^j\Gamma(s/2+j)}{(j!)^2\Gamma(1-s/2-j)}W_{2n-1}(-(2j+s)) = -\frac{\Gamma(s/2)}{\Gamma(1-s/2)}\binom{-s/2}{j}^2 W_{2n-1}(-s-2j).$$

Thus it follows that

$$W_{2n}(-s) = \sum_{j\geqslant 0}\binom{-s/2}{j}^2 W_{2n-1}(-s-2j), \tag{3.68}$$

which is what we want to prove, provided that the contour of the integral after (3.67) can be closed in the right half-plane. This is Conjecture 3.4.2 below. □

This proof is thus rigorous provided that the next two conjectures hold. However, note that Conjecture 3.4.1 is easily checked for individual n. In particular, it is true for $2n-1\leqslant 45$.

Conjecture 3.4.1 (Poles of W_{2n-1})**.** *For each $n \geqslant 1$ all poles of W_{2n-1} are simple.*

Conjecture 3.4.2 (Growth of W_{2n-1})**.** *For given s,*

$$\liminf_{r\to\infty} \int_{\gamma_r} \frac{\Gamma(z/2)\Gamma(s/2-z/2)}{\Gamma(1-z/2)\Gamma(1-s/2+z/2)} W_{2n-1}(-z)\,\mathrm{d}z = 0,$$

where γ_r is a right half-circle of radius r around $\delta \in (0,1)$.

Remark 3.4.3 (Other approaches to Conjecture 3.1.1)**.** We restrict ourself to the core case with $n = 2$. One can prove that both sides of the needed identity satisfy the recursion for W_4. Hence, it suffices to show that the conjecture is correct for $s = \pm 1$. Working entirely formally with (3.11) and ignoring the restriction on s we have:

$$\begin{aligned}
\sum_{j\geqslant 0} \binom{-1/2}{j}^2 W_3(-1-2j) &= \sum_{j=0}^{\infty} \binom{-1/2}{j}^2 2^{-2j} \frac{\Gamma(\frac{1}{2}-j)}{\Gamma(\frac{1}{2}+j)} \int_0^\infty x^{2j} J_0^3(x)\,\mathrm{d}x \\
&= \int_0^\infty J_0^3(x) \sum_{j=0}^{\infty} \binom{-1/2}{j}^2 \frac{\Gamma(\frac{1}{2}-j)}{\Gamma(\frac{1}{2}+j)} \left(\frac{x}{2}\right)^{2j} \mathrm{d}x \\
&= \int_0^\infty J_0^4(x)\,\mathrm{d}x \\
&= W_4(-1),
\end{aligned}$$

on appealing to Example 3.2.1, since

$$\sum_{j=0}^{\infty} \binom{-1/2}{j}^2 \frac{\Gamma(\frac{1}{2}-j)}{\Gamma(\frac{1}{2}+j)} x^{2j} = J_0(2x)$$

for $x > 0$. There is a corresponding manipulation for $s = 1$, but we cannot make them rigorous. However, in [BSWZ11], we prove the conjecture for $n = 2$ and s an integer. $\Diamond$

Conclusion

In addition to the two new conjectures made explicit above, it would be fascinating to obtain closed forms for any of the residues in Proposition 3.2.4 with $n \geqslant 5$. It would likewise be very informative to obtain a closed form for $W_5(\pm 1)$.

Chapter 4

Densities of short uniform random walks

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[BSWZ11] *Densities of short uniform random walks*
(with Jonathan M. Borwein, James Wan, Wadim Zudilin (appendix by Don Zagier))
to appear in Canadian Journal of Mathematics

Abstract We study the densities of uniform random walks in the plane. A special focus is on the case of short walks with three or four steps and less completely those with five steps. As one of the main results, we obtain a hypergeometric representation of the density for four steps, which complements the classical elliptic representation in the case of three steps. It appears unrealistic to expect similar results for more than five steps. New results are also presented concerning the moments of uniform random walks and, in particular, their derivatives. Relations with Mahler measures are discussed.

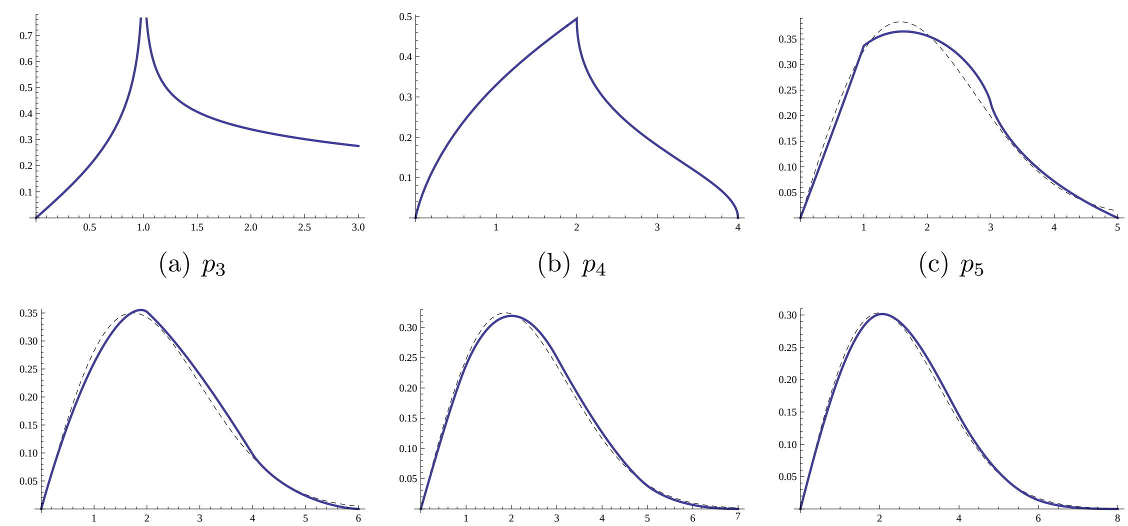
4.1 Introduction

An n-step uniform random walk is a walk in the plane that 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 [Pea05a, Pea05b, Pea06] who posed the problem of determining the distribution of the distance from the origin after a certain number of steps. In this paper, we study the (radial) densities p_n of the distance travelled in n steps. This continues research commenced in [BNSW11, BSW11] where the focus was on the moments of these distributions:

$$W_n(s) := \int_0^n p_n(t) t^s \,\mathrm{d}t.$$

The densities for walks of up to 8 steps are depicted in Figure 4.1. As established by Lord Rayleigh [Ray05], p_n quickly approaches the probability density $\frac{2x}{n}e^{-x^2/n}$ for large n. This limiting density is superimposed in Figure 4.1 for $n \geqslant 5$.



(a) p_3 (b) p_4 (c) p_5

(d) p_6 (e) p_7 (f) p_8

Figure 4.1: Densities p_n with the limiting behaviour superimposed for $n \geqslant 5$.

Closed forms were only known in the cases $n = 2$ and $n = 3$. The evaluation, for $0 \leqslant x \leqslant 2$,

$$p_2(x) = \frac{2}{\pi\sqrt{4-x^2}} \tag{4.1}$$

is elementary. On the other hand, the density $p_3(x)$ for $0 \leqslant x \leqslant 3$ can be expressed in terms of elliptic integrals by

$$p_3(x) = \operatorname{Re}\left(\frac{\sqrt{x}}{\pi^2}\,K\left(\sqrt{\frac{(x+1)^3(3-x)}{16x}}\right)\right), \tag{4.2}$$

see, e.g., [Pea06]. One of the main results of this paper is a closed form evaluation of p_4 as a hypergeometric function given in Theorem 4.4.9. In (4.20) we also provide a single hypergeometric closed form for p_3 which, in contrast to (4.2), is real and valid on all of $[0,3]$. For convenience, we list these two closed forms here:

$$p_3(x) = \frac{2\sqrt{3}}{\pi}\,\frac{x}{(3+x^2)}\,{}_2F_1\left(\left.\begin{matrix}\frac{1}{3},\frac{2}{3}\\ 1\end{matrix}\,\right|\,\frac{x^2\left(9-x^2\right)^2}{\left(3+x^2\right)^3}\right), \tag{4.3}$$

$$p_4(x) = \frac{2}{\pi^2}\,\frac{\sqrt{16-x^2}}{x}\,\operatorname{Re}\,{}_3F_2\left(\left.\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{5}{6},\frac{7}{6}\end{matrix}\,\right|\,\frac{\left(16-x^2\right)^3}{108x^4}\right). \tag{4.4}$$

We note that while *Maple* handled these well to high precision, *Mathematica* struggled, especially with the analytic continuation of the ${}_3F_2$ when the argument is greater than 1.

A striking feature of the 3- and 4-step random walk densities is their modularity. It is this circumstance which not only allows us to express them via hypergeometric series, but also makes them a remarkable object of mathematical study.

This paper is structured as follows: In Section 4.2 we give general results for the densities p_n and prove for instance that they satisfy certain linear differential equations. In Sections 4.3, 4.4, and 4.5 we provide special results for p_3, p_4, and p_5 respectively. Particular interest is taken in the behaviour near the points where the densities fail to be smooth. In Section 4.6 we study the derivatives of the moment function and make a connection to multidimensional Mahler measures. Finally in Section 4.7 we provide some related new evaluations of moments and so resolve a central case of an earlier conjecture on convolutions of moments in [BSW11].

The amazing story of the appearance of Theorem 4.2.7 is worth mentioning here. The theorem was a conjecture in an earlier version of this manuscript, and one of the present authors communicated it to D. Zagier. That author was surprised to learn that Zagier had already been asked for a proof of exactly the same identities a little earlier, by P. Djakov and B. Mityagin.

Those authors had in fact proved the theorem already in 2004 (see [DM04, Theorem 4.1] and [DM07, Theorem 8]) during their study of the asymptotics of the spectral gaps of a Schrödinger operator with a two-term potential — their proof was indirect, so that we should never have come across the identities without the accident of asking the same person the same question! Djakov and Mityagin asked Zagier about the possibility of a direct proof of their identities (the subject of Theorem 4.2.7), and he gave a very neat and purely combinatorial answer. It is this proof which is herein presented in the Appendix.

We close this introduction with a historical remark illustrating the fascination arising from these densities and their curious geometric features. H. Fettis devotes the entire paper [Fet63] to proving that p_5 is not linear on the initial interval $[0, 1]$ as ruminated upon by Pearson [Pea06]. This will be explained in Section 4.5.

4.2 The densities p_n

It is a classical result of Kluyver [Klu06] that p_n has the following Bessel integral representation:

$$p_n(x) = \int_0^\infty xtJ_0(xt)J_0^n(t)\,\mathrm{d}t. \tag{4.5}$$

Here J_ν is the *Bessel function of the first kind* of order ν.

Remark 4.2.1. Equation (4.5) naturally generalizes to the case of nonuniform step lengths. In particular, for $n = 2$ and step lengths a and b we record (see [Wat41,

p. 411] or [Hug95, 2.3.2]; the result is attributed to Sonine) that the corresponding density is

$$
\begin{aligned}
p_2(x; a, b) &= \int_0^\infty xt J_0(xt) J_0(at) J_0(bt)\, \mathrm{d}t \\
&= \frac{2x}{\pi\sqrt{((a+b)^2 - x^2)(x^2 - (a-b)^2)}}
\end{aligned} \tag{4.6}
$$

for $|a - b| \leqslant x \leqslant a + b$ and $p_2(x; a, b) = 0$ otherwise. Observe how (4.6) specializes to (4.1) in the case $a = b = 1$.

In the case $n = 3$ the density $p_3(x; a, b, c)$ has been evaluated by Nicholson [Wat41, p. 414] in terms of elliptic integrals directly generalizing (4.2). The corresponding extensions for four and more variables appear much less accessible. ♢

It is visually clear from the graphs in Figure 4.1 that p_n is getting smoother for increasing n. This can be made precise from (4.5) using the asymptotic formula for J_0 for large arguments and dominated convergence:

Theorem 4.2.2. *For each integer $n \geqslant 0$, the density p_{n+4} is $\lfloor n/2 \rfloor$ times continuously differentiable.*

On the other hand, we note from Figure 4.1 that the only points preventing p_n from being smooth appear to be integers. This will be made precise in Theorem 4.2.4.

To this end, we recall a few things about the s-th moments $W_n(s)$ of the density p_n which are given by

$$
W_n(s) = \int_0^\infty x^s p_n(x)\, \mathrm{d}x = \int_{[0,1]^n} \left| \sum_{k=1}^n e^{2\pi x_k i} \right|^s \mathrm{d}\boldsymbol{x}. \tag{4.7}
$$

Starting with the right-hand side, these moments had been investigated in [BNSW11, BSW11]. There it was shown that $W_n(s)$ admits an *analytic continuation* to all of the complex plane with poles of at most order two at certain negative integers. In particular, $W_3(s)$ has simple poles at $s = -2, -4, -6, \ldots$ and $W_4(s)$ has double poles at these integers [BNSW11, Thm. 6, Ex. 2 & 3].

Moreover, from the combinatorial evaluation

$$W_n(2k) = \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2 \tag{4.8}$$

for integers $k \geqslant 0$ it followed that $W_n(s)$ satisfies a functional equation, as in [BNSW11, Ex. 1], coming from the inevitable recursion that exists for the right-hand side of (4.8) . For instance,

$$(s+4)^2 W_3(s+4) - 2(5s^2+30s+46)W_3(s+2) + 9(s+2)^2 W_3(s) = 0,$$

and equation (4.9) below.

The first part of equation (4.7) can be rephrased as saying that $W_n(s-1)$ is the *Mellin transform* of p_n ([ML86]). We denote this by $W_n(s-1) = \mathcal{M}\left[p_n; s\right]$. Conversely, the density p_n is the *inverse Mellin transform* of $W_n(s-1)$. We intend to exploit this relation as detailed for $n = 4$ in the following example.

Example 4.2.3 (Mellin transforms)**.** For $n = 4$, the moments $W_4(s)$ satisfy the functional equation

$$(s+4)^3 W_4(s+4) - 4(s+3)(5s^2+30s+48)W_4(s+2) + 64(s+2)^3 W_4(s) = 0. \tag{4.9}$$

Recall the following rules for the Mellin transform: if $F(s) = \mathcal{M}\left[f; s\right]$ then in the appropriate strips of convergence

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

Here, and below, D_x denotes differentiation with respect to x, and, for the second rule to be true, we have to assume, for instance, that f is continuously differentiable.

Thus, purely formally, we can translate the functional equation (4.9) of W_4 into the differential equation $A_4 \cdot p_4(x) = 0$ where A_4 is the operator

$$A_4 = x^4(\theta+1)^3 - 4x^2\theta(5\theta^2+3) + 64(\theta-1)^3 \tag{4.10}$$

$$= (x-4)(x-2)x^3(x+2)(x+4)D_x^3 + 6x^4\left(x^2-10\right)D_x^2 \tag{4.11}$$

$$+ x\left(7x^4 - 32x^2 + 64\right)D_x + \left(x^2-8\right)\left(x^2+8\right).$$

Here $\theta = xD_x$. However, it should be noted that p_4 is not continuously differentiable. Moreover, $p_4(x)$ is approximated by a constant multiple of $\sqrt{4-x}$ as $x \to 4^-$ (see Theorem 4.4.1) so that the second derivative of p_4 is not even locally integrable. In particular, it does not have a Mellin transform in the classical sense. $\diamondsuit$

Theorem 4.2.4. *Let an integer $n \geqslant 1$ be given.*

- *The density p_n satisfies a differential equation of order $n-1$.*
- *If n is even (respectively odd) then p_n is real analytic except at 0 and the even (respectively odd) integers $m \leq n$.*

Proof. As illustrated for p_4 in Example 4.2.3, we formally use the Mellin transform method to translate the functional equation of W_n into a differential equation $A_n \cdot y(x) = 0$. Since p_n is locally integrable and compactly supported, it has a Mellin transform in the distributional sense as detailed for instance in [ML86]. It follows rigorously that p_n solves $A_n \cdot y(x) = 0$ in a distributional sense. In other words, p_n is a weak solution of this differential equation. The degree of this equation is $n-1$ because the functional equation satisfied by W_n has coefficients of degree $n-1$ as shown in [BNSW11, Thm. 1].

The leading coefficient of the differential equation (in terms of D_x as in (4.11)) turns out to be

$$x^{n-1} \prod_{2|(m-n)} (x^2 - m^2) \tag{4.12}$$

where the product is over the even or odd integers $1 \leq m \leq n$ depending on whether n is even or odd. This is discussed below in Section 4.2.1.

Thus the leading coefficient of the differential equation is nonzero on $[0, n]$ except for 0 and the even or odd integers already mentioned. On each interval not containing these points it follows, as described for instance in [Hör89, Cor. 3.1.6], that p_n is in fact a classical solution of the differential equation. Moreover the analyticity of the coefficients, which are polynomials in our case, implies that p_n is piecewise real analytic as claimed. □

Remark 4.2.5. It is one of the basic properties of the Mellin transform, see for instance [FS09, Appendix B.7], that 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. It is shown in [BNSW11] that the poles of $W_n(s)$ occur at specific negative integers and are at most of second order. This translates into the fact that p_n has an expansion at 0 as a power series with additional logarithmic terms in the presence of double poles. This is made explicit in the case of p_4 in Example 4.4.3.

4.2.1 An explicit recursion

We close this section by providing details for the claim made in (4.12). Recall that the even moments $f_n(k) := W_n(2k)$ satisfy a recurrence of order $\lambda := \lceil n/2 \rceil$ with polynomial coefficients of degree $n - 1$ (see [BNSW11]). An entirely explicit formula for this recurrence is given in [Ver04]:

Theorem 4.2.6.

$$\sum_{j\geqslant 0}\left[k^{n+1}\sum_{\alpha_1,\ldots,\alpha_j}\prod_{i=1}^{j}(-\alpha_i)(n+1-\alpha_i)\left(\frac{k-i}{k-i+1}\right)^{\alpha_i-1}\right]f_n(k-j)=0 \tag{4.13}$$

where the sum is over all sequences $\alpha_1,\ldots,\alpha_j$ *such that* $0\leqslant\alpha_i\leqslant n$ *and* $\alpha_{i+1}\leqslant\alpha_i-2$.

Observe that (4.12) is easily checked for each fixed n by applying Theorem 4.2.6. We explicitly checked the cases $n\leqslant 1000$ (using a recursive formulation of Theorem 4.2.6 from [Ver04]) while only using this statement for $n\leqslant 5$ in this paper. The fact that (4.12) is true in general is recorded and made more explicit in Theorem 4.2.7 below.

For fixed n, write the recurrence for $f_n(k)$ in the form $\sum_{j=0}^{n-1}k^jq_j(K)$ where q_j are polynomials and K is the shift $k\to k+1$. Then q_{n-1} is the characteristic polynomial of this recurrence, and, by the rules outlined in Example 4.2.3, we find that the differential equation satisfied by $p_n(x)$ is of the form $q_{n-1}(x^2)\theta^{n-1}+\cdots$, where $\theta=xD_x$ and the dots indicate terms of lower order in θ.

We claim that the characteristic polynomial of the recurrence (4.13) satisfied by $f_n(k)$ is $\prod_{2|(m-n)}(x-m^2)$ where the product is over the integers $1\leq m\leq n$ such that $m\equiv n$ modulo 2. This implies (4.12). By Theorem 4.2.6 the characteristic polynomial is

$$\sum_{j=0}^{\lambda}\left[\sum_{\alpha_1,\ldots,\alpha_j}\prod_{i=1}^{j}(-\alpha_i)(n+1-\alpha_i)\right]x^{\lambda-j} \tag{4.14}$$

where $\lambda=\lceil n/2\rceil$ and the sum is again over all sequences $\alpha_1,\ldots,\alpha_j$ such that $0\leqslant\alpha_i\leqslant n$ and $\alpha_{i+1}\leqslant\alpha_i-2$. The claimed evaluation is thus equivalent to the following identity, first proven by P. Djakov and B. Mityagin [DM04, DM07]. Zagier's more direct and purely combinatorial proof is given in the Appendix.

Theorem 4.2.7. *For all integers $n, j \geqslant 1$,*

$$\sum_{\substack{0\leqslant m_1,\ldots,m_j<n/2\\ m_i<m_{i+1}}} \prod_{i=1}^{j} (n-2m_i)^2 = \sum_{\substack{1\leqslant \alpha_1,\ldots,\alpha_j\leqslant n\\ \alpha_i\leqslant \alpha_{i+1}-2}} \prod_{i=1}^{j} \alpha_i(n+1-\alpha_i). \tag{4.15}$$

4.3 The density p_3

The elliptic integral evaluation (4.2) of p_3 is very suitable to extract information about the features of p_3 exposed in Figure 4.1(a). It follows, for instance, that p_3 has a singularity at 1. Moreover, using the known asymptotics for $K(x)$, we may deduce that the singularity is of the form

$$p_3(x) = \frac{3}{2\pi^2} \log\left(\frac{4}{|x-1|}\right) + O(1) \tag{4.16}$$

as $x \to 1$.

We also recall from [BSW11, Ex. 5] that p_3 has the expansion, valid for $0 \leqslant x \leqslant 1$,

$$p_3(x) = \frac{2x}{\pi\sqrt{3}} \sum_{k=0}^{\infty} W_3(2k) \left(\frac{x}{3}\right)^{2k} \tag{4.17}$$

where

$$W_3(2k) = \sum_{j=0}^{k} \binom{k}{j}^2 \binom{2j}{j} \tag{4.18}$$

is the sum of squares of trinomials. Moreover, we have from [BSW11, Eqn. 29] the functional relation

$$p_3(x) = \frac{4x}{(3-x)(x+1)}\, p_3\left(\frac{3-x}{1+x}\right) \tag{4.19}$$

so that (4.17) determines p_3 completely and also makes apparent the behaviour at 3.

We close this section with two more alternative expressions for p_3.

Example 4.3.1 (Hypergeometric form for p_3)**.** Using the techniques in [CZ10] we can deduce from (4.17) that

$$p_3(x) = \frac{2\sqrt{3}x}{\pi\,(3+x^2)}\,{}_2F_1\left(\frac{1}{3}, \frac{2}{3};\ 1;\ \frac{x^2\,(9-x^2)^2}{(3+x^2)^3}\right) \tag{4.20}$$

which is found in a similar but simpler way than the hypergeometric form of p_4 given in Theorem 4.4.9. Once obtained, this identity is easily proven using the differential equation from Theorem 4.2.4 satisfied by p_3. From (4.20) we see, for example, that $p_3(\sqrt{3})^2 = \frac{3}{2\pi^2}W_3(-1)$. $\Diamond$

Example 4.3.2 (Iterative form for p_3)**.** The expression (4.20) can be interpreted in terms of the cubic AGM, AG_3, see [BB91], as follows. Recall that $\mathrm{AG}_3(a,b)$ is 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 $b_0 = b$. The iterations converge cubically, thus allowing for very efficient high-precision evaluation. On the other hand,

$$\frac{1}{\mathrm{AG}_3(1,s)} = {}_2F_1\left(\frac{1}{3}, \frac{2}{3}; 1; 1-s^3\right)$$

so that in consequence of (4.20), for $0 \leqslant x \leqslant 3$,

$$p_3(x) = \frac{2\sqrt{3}}{\pi}\,\frac{x}{\mathrm{AG}_3(3+x^2, 3\,|1-x^2|^{2/3})}. \tag{4.21}$$

Note that $p_3(3) = \frac{\sqrt{3}}{2\pi}$ is a direct consequence of the final formula.

Finally we remark that the cubic AGM also makes an appearance in the case $n = 4$. We just mention that the modular properties of p_4 recorded in Remark 4.4.11

can be stated in terms of the theta functions

$$b(\tau) = \frac{\eta(\tau)^3}{\eta(3\tau)}, \quad c(\tau) = 3\frac{\eta(3\tau)^3}{\eta(\tau)} \tag{4.22}$$

where η is the Dedekind eta function defined in (4.42). For more information and proper definitions of the functions b, c as well as a, which is related by $a^3 = b^3 + c^3$, we refer to [BBG94]. Ultimately we are hopeful that, in search for an analogue of (4.19) for p_4, this may lead to an algebraic relation between algebraically related arguments of p_4. $\diamondsuit$

4.4 The density p_4

The densities p_n are recursively related. As in [Hug95], setting $\phi_n(x) = p_n(x)/(2\pi x)$, we have that for integers $n \geqslant 2$

$$\phi_n(x) = \frac{1}{2\pi} \int_0^{2\pi} \phi_{n-1}\left(\sqrt{x^2 - 2x\cos\alpha + 1}\right) \mathrm{d}\alpha. \tag{4.23}$$

We use this recursive relation to get some quantitative information about the behaviour of p_4 at $x = 4$.

Theorem 4.4.1. *As $x \to 4^-$,*

$$p_4(x) = \frac{\sqrt{2}}{\pi^2}\sqrt{4-x} - \frac{3\sqrt{2}}{16\pi^2}(4-x)^{3/2} + \frac{23\sqrt{2}}{512\pi^2}(4-x)^{5/2} + O\left((4-x)^{7/2}\right).$$

Proof. Set $y = \sqrt{x^2 - 2x\cos\alpha + 1}$. For $2 < x < 4$,

$$\phi_4(x) = \frac{1}{\pi}\int_0^{\pi} \phi_3(y)\,\mathrm{d}\alpha = \frac{1}{\pi}\int_0^{\arccos\left(\frac{x^2-8}{2x}\right)} \phi_3(y)\,\mathrm{d}\alpha$$

since ϕ_3 is only supported on $[0, 3]$. Note that $\phi_3(y)$ is continuous and bounded in the domain of integration. By the Leibniz integral rule, we can thus differentiate under the integral sign to obtain

$$\phi_4'(x) = -\frac{1}{\pi}\frac{(x^2+8)\,\phi_3(3)}{x\sqrt{(16-x^2)(x^2-4)}} + \frac{1}{\pi}\int_0^{\arccos(\frac{x^2-8}{2x})} (x - \cos(\alpha))\,\frac{\phi_3'(y)}{y}\,\mathrm{d}\alpha. \tag{4.24}$$

This shows that ϕ_4', and hence p_4', have a singularity at $x = 4$. More specifically,

$$\phi_4'(x) = -\frac{1}{8\sqrt{2}\pi^3\sqrt{4-x}} + O(1) \quad \text{as } x \to 4^-.$$

Here, we used that $\phi_3(3) = \frac{\sqrt{3}}{12\pi^2}$. It follows that

$$p_4'(x) = -\frac{1}{\sqrt{2}\pi^2\sqrt{4-x}} + O(1)$$

which, upon integration, is the claim to first order. Differentiating (4.24) twice more proves the claim. $\square$

Remark 4.4.2. The situation for the singularity at $x = 2^+$ is more complicated since in (4.24) both the integral (via the logarithmic singularity of ϕ_3 at 1, see (4.16)) and the boundary term contribute. Numerically, we find, as $x \to 2^+$,

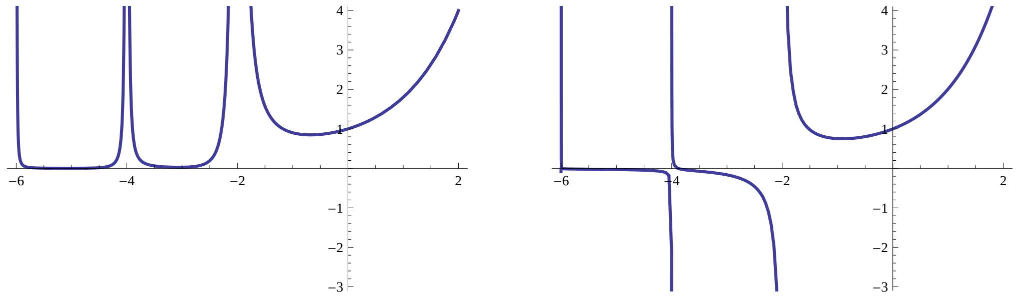
$$p_4'(x) = -\frac{2}{\pi^2\sqrt{x-2}} + O(1).$$

On the other hand, the derivative of p_4 at 2 from the left is given by

$$p_4'(2^-) = \frac{\sqrt{3}}{\pi}\,{}_3F_2\left(\left.\begin{matrix} -\frac{1}{2}, \frac{1}{3}, \frac{2}{3} \\ 1, 1 \end{matrix}\right| 1\right) - \frac{2}{3}\,p_4(2).$$

These observations can be proven in hindsight from Theorem 4.4.7. $\lozenge$

We now turn to the behaviour of p_4 at zero which we derive from the pole structure of W_4 as described in Remark 4.2.5.



(a) W_4 (b) W_5

Figure 4.2: W_4 and W_5 analytically continued to the real line.

Example 4.4.3. From [BSW11], we know that W_4 has a pole of order 2 at -2 as illustrated in Figure 4.2(a). More specifically, results in Section 4.6 give

$$W_4(s) = \frac{3}{2\pi^2}\frac{1}{(s+2)^2} + \frac{9}{2\pi^2}\log(2)\frac{1}{s+2} + O(1)$$

as $s \to -2$. It therefore follows that

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

as $x \to 0$. $\Diamond$

More generally, W_4 has poles of order 2 at $-2k$ for k a positive integer. Define $s_{4,k}$ and $r_{4,k}$ by

$$W_4(s) = \frac{s_{4,k-1}}{(s+2k)^2} + \frac{r_{4,k-1}}{s+2k} + O(1) \tag{4.25}$$

as $s \to -2k$. We thus obtain that, as $x \to 0^+$,

$$p_4(x) = \sum_{k=0}^{K-1} x^{2k+1}\left(r_{4,k} - s_{4,k}\log(x)\right) + O(x^{2K+1}).$$

In fact, knowing that p_4 solves the linear Fuchsian differential equation (4.10) with a regular singularity at 0 we may conclude:

Theorem 4.4.4. *For small values $x > 0$,*

$$p_4(x) = \sum_{k=0}^{\infty} \left(r_{4,k} - s_{4,k} \log(x)\right) x^{2k+1}. \tag{4.26}$$

Note that

$$s_{4,k} = \frac{3}{2\pi^2} \frac{W_4(2k)}{8^{2k}}$$

as the two sequences satisfy the same recurrence and initial conditions. The numbers $W_4(2k)$ are also known as the Domb numbers ([BBBG08]), and their generating function in hypergeometric form is given in [Rog09] and has been further studied in [CZ10]. We thus have

$$\sum_{k=0}^{\infty} s_{4,k}\, x^{2k+1} = \frac{6x}{\pi^2\,(4-x^2)}\, {}_3F_2\left(\left.{\frac{1}{3}, \frac{1}{2}, \frac{2}{3} \atop 1, 1}\right| \frac{108x^2}{(x^2-4)^3}\right) \tag{4.27}$$

which is readily verified to be an analytic solution to the differential equation satisfied by p_4.

Remark 4.4.5. For future use, we note that (4.27) can also be written as

$$\sum_{k=0}^{\infty} s_{4,k}\, x^{2k+1} = \frac{24x}{\pi^2\,(16-x^2)}\, {}_3F_2\left(\left.{\frac{1}{3}, \frac{1}{2}, \frac{2}{3} \atop 1, 1}\right| \frac{108x^4}{(16-x^2)^3}\right) \tag{4.28}$$

which follows from the transformation

$$(1-4x)\,{}_3F_2\left(\left.{\frac{1}{3}, \frac{1}{2}, \frac{2}{3} \atop 1, 1}\right| -\frac{108x}{(1-16x)^3}\right) = (1-16x)\,{}_3F_2\left(\left.{\frac{1}{3}, \frac{1}{2}, \frac{2}{3} \atop 1, 1}\right| \frac{108x^2}{(1-4x)^3}\right) \tag{4.29}$$

given in [CZ10, (3.1)]. $\diamondsuit$

On the other hand, as a consequence of (4.25) and the functional equation (4.9) satisfied by W_4, the residues $r_{4,k}$ can be obtained from the recurrence relation

$$128k^3 r_{4,k} = 4(2k-1)(5k^2-5k+2)r_{4,k-1} - 2(k-1)^3 r_{4,k-2} + 3\left(64k^2 s_{4,k} - (20k^2-20k+6)s_{4,k-1} + (k-1)^2 s_{4,k-2}\right) \tag{4.30}$$

with $r_{4,-1}=0$ and $r_{4,0} = \frac{9}{2\pi^2}\log(2)$.

Remark 4.4.6. In fact, before realizing the connection between the Mellin transform and the behaviour of p_4 at 0, we empirically found that p_4 on $(0,2)$ should be of the form $r(x) - s(x)\log(x)$ where a and r are odd and analytic. We then numerically determined the coefficients and observed the relation with the residues of W_4 as given in Theorem 4.4.4. $\Diamond$

The differential equation for p_4 has a regular singularity at 0. A basis of solutions at 0 can therefore be obtained via the Frobenius method, see for instance [Inc26]. Since the indicial equation has 1 as a triple root, the solution (4.27) is the unique analytic solution at 0 while the other solutions have a logarithmic or double logarithmic singularity. The solution with a logarithmic singularity at 0 is explicitly given in (4.34), and, from (4.26), it is clear that p_4 on $(0,2)$ is a linear combination of the analytic and the logarithmic solution.

Moreover, the differential equation for p_4 is a symmetric square. In other words, it can be reduced to a second order differential equation, which after a quadratic substitution, has 4 regular singularities and is thus of Heun type. In fact, a hypergeometric representation of p_4 with rational argument is possible.

Theorem 4.4.7. *For $2 < x < 4$,*

$$p_4(x) = \frac{2}{\pi^2}\frac{\sqrt{16-x^2}}{x}\,{}_3F_2\left(\left.\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{5}{6},\frac{7}{6}\end{matrix}\,\right|\,\frac{(16-x^2)^3}{108x^4}\right). \tag{4.31}$$

Proof. Denote the right-hand side of (4.31) by $q_4(x)$ and observe that the hypergeometric series converges for $2 < x < 4$. It is routine to verify that q_4 is a solution of the differential equation $A_4 \cdot y(x) = 0$ given in (4.10) which is also satisfied by p_4 as proven in Theorem 4.2.4. Together with the boundary conditions supplied by Theorem 4.4.1 it follows that $p_4 = q_4$. □

We note that Theorem 4.4.7 gives $2\sqrt{16-x^2}/(\pi^2 x)$ as an approximation to $p_4(x)$ near $x = 4$, which is much more accurate than the elementary estimates established in Theorem 4.4.1.

Corollary 4.4.8. *In particular,*

$$p_4(2) = \frac{2^{7/3}\pi}{3\sqrt{3}}\,\Gamma\left(\frac{2}{3}\right)^{-6} = \frac{\sqrt{3}}{\pi}\,W_3(-1). \tag{4.32}$$

Quite marvelously, as first discovered numerically:

Theorem 4.4.9. *For $0 < x < 4$,*

$$p_4(x) = \frac{2}{\pi^2}\,\frac{\sqrt{16-x^2}}{x}\,\operatorname{Re}\,{}_3F_2\left(\left.\begin{matrix}\frac{1}{2},\frac{1}{2},\frac{1}{2}\\ \frac{5}{6},\frac{7}{6}\end{matrix}\right|\frac{\left(16-x^2\right)^3}{108x^4}\right). \tag{4.33}$$

Proof. To obtain the analytic continuation of the ${}_3F_2$ for $0 < x < 2$ we employ the formula [Luk69, 5.3], valid for all z,

$$\begin{aligned}{}_{q+1}F_q\left(\left.\begin{matrix}a_1,\dots,a_{q+1}\\ b_1,\dots,b_q\end{matrix}\right|z\right) &= \frac{\prod_j\Gamma(b_j)}{\prod_j\Gamma(a_j)}\sum_{k=1}^{q+1}\frac{\Gamma(a_k)\prod_{j\neq k}\Gamma(a_j-a_k)}{\prod_j\Gamma(b_j-a_k)}(-z)^{-a_k}\\ &\quad\times{}_{q+1}F_q\left(\left.\begin{matrix}a_k,\{a_k-b_j+1\}_j\\ \{a_k-a_j+1\}_{j\neq k}\end{matrix}\right|\frac{1}{z}\right),\end{aligned}$$

which requires the a_j to not differ by integers. Therefore we apply it to

$${}_3F_2\left(\left.\begin{matrix}\frac{1}{2}+\varepsilon,\frac{1}{2},\frac{1}{2}-\varepsilon\\ \frac{5}{6},\frac{7}{6}\end{matrix}\right|z\right).$$

and take the limit as $\varepsilon \to 0$. This ultimately produces, for $z > 1$,

$$\operatorname{Re}\, {}_3F_2\left(\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\\ \frac{5}{6}, \frac{7}{6}\end{matrix}\middle| z\right) = \frac{\log(108z)}{2\sqrt{3z}}\, {}_3F_2\left(\begin{matrix}\frac{1}{3}, \frac{1}{2}, \frac{2}{3}\\ 1, 1\end{matrix}\middle| \frac{1}{z}\right) + \frac{1}{2\sqrt{3z}} \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{1}{2})_n (\frac{2}{3})_n}{n!^3} \left(\frac{1}{z}\right)^n (5H_n - 2H_{2n} - 3H_{3n}). \tag{4.34}$$

Here $H_n = \sum_{k=1}^n 1/k$ is the n-th harmonic number. Now, insert the appropriate argument for z and the factors so the left-hand side corresponds to the claimed closed form. Observing that

$$\left(\tfrac{1}{3}\right)_n \left(\tfrac{1}{2}\right)_n \left(\tfrac{2}{3}\right)_n = \frac{(2n)!(3n)!}{108^n (n!)^2},$$

we thus find that the right-hand side of (4.33) is given by $-\log(x)S_4(x)$ plus

$$\frac{6}{\pi^2} \sum_{n=0}^{\infty} \frac{(2n)!(3n)!}{(n!)^5} \frac{x^{4n+1}}{(16 - x^2)^{3n}} \left(5H_n - 2H_{2n} - 3H_{3n} + 3\log(16 - x^2)\right)$$

where S_4 is the solution (analytic at 0) to the differential equation for p_4 given in (4.28). This combination can now be verified to be a formal and hence actual solution of the differential equation for p_4. Together with the boundary conditions supplied by Theorem 4.4.4 this proves the claim. □

Remark 4.4.10. Let us indicate how the hypergeometric expression for p_4 given in Theorem 4.4.7 was discovered. Consider the generating series

$$y_0(z) = \sum_{k=0}^{\infty} W_4(2k) z^k \tag{4.35}$$

of the Domb numbers which is just a rescaled version of (4.27). Corresponding to (4.28), the hypergeometric form for this series given in [Rog09] is

$$y_0(z) = \frac{1}{1 - 4z}\, {}_3F_2\left(\begin{matrix}\frac{1}{3}, \frac{1}{2}, \frac{2}{3}\\ 1, 1\end{matrix}\middle| \frac{108z^2}{(1 - 4z)^3}\right) \tag{4.36}$$

which converges for $|z| < 1/16$. y_0 satisfies the differential equation $B_4 \cdot y_0(z) = 0$ where

$$B_4 = 64z^2(\theta+1)^3 - 2z(2\theta+1)(5\theta^2+5\theta+2) + \theta^3 \tag{4.37}$$

and $\theta = z\frac{\mathrm{d}}{\mathrm{d}z}$. Up to a change of variables this is (4.10); y_0 is the unique solution which is analytic at zero and takes the value 1 at zero; the other solutions which are not a multiple of y_0 have a single or double logarithmic singularity. Let y_1 be the solution characterized by

$$y_1(z) - y_0(z)\log(z) \in z\mathbb{Q}[[z]]. \tag{4.38}$$

Note that it follows from (4.38) as well as Theorem 4.4.4 together with the initial values $s_{4,0} = \frac{3}{2\pi^2}$ and $r_{4,0} = s_{4,0}\log(8)$ that p_4, for small positive argument, is given by

$$p_4(x) = -\frac{3x}{4\pi^2}\, y_1\left(\frac{x^2}{64}\right). \tag{4.39}$$

If $x \in (2,4)$ and $z = x^2/64$ then the argument $t = \frac{108z^2}{(1-4z)^3}$ of the hypergeometric function in (4.36) takes the values $(1,\infty)$. We therefore consider the solutions of the corresponding hypergeometric equation at infinity. A standard basis for these is

$$t^{-1/3}{}_3F_2\left(\begin{matrix}\frac13,\frac13,\frac13\\ \frac23,\frac56\end{matrix}\middle|\frac1t\right),\quad t^{-1/2}{}_3F_2\left(\begin{matrix}\frac12,\frac12,\frac12\\ \frac56,\frac76\end{matrix}\middle|\frac1t\right),\quad t^{-2/3}{}_3F_2\left(\begin{matrix}\frac23,\frac23,\frac23\\ \frac43,\frac76\end{matrix}\middle|\frac1t\right). \tag{4.40}$$

In fact, the second element suffices to express p_4 on the interval $(2,4)$ as shown in Theorem 4.4.7. ◊

We close this section by showing that, remarkably, p_4 has modular structure.

Remark 4.4.11. As shown in [CZ10] the series y_0 defined in (4.35) possesses the modular parameterization

$$y_0\left(-\frac{\eta(2\tau)^6\eta(6\tau)^6}{\eta(\tau)^6\eta(3\tau)^6}\right)=\frac{\eta(\tau)^4\eta(3\tau)^4}{\eta(2\tau)^2\eta(6\tau)^2}. \tag{4.41}$$

Here η is the *Dedekind eta function* defined as

$$\eta(\tau)=q^{1/24}\prod_{n=1}^{\infty}(1-q^n)=q^{1/24}\sum_{n=-\infty}^{\infty}(-1)^n q^{n(3n+1)/2}, \tag{4.42}$$

where $q=e^{2\pi i\tau}$. Moreover, the quotient of the logarithmic solution y_1 defined in (4.38) and y_0 is related to the modular parameter τ used in (4.41) by

$$\exp\left(\frac{y_1(z)}{y_0(z)}\right)=e^{(2\tau+1)\pi i}=-q. \tag{4.43}$$

Combining (4.41), (4.43) and (4.39) one obtains the modular representation

$$p_4\left(8i\frac{\eta(2\tau)^3\eta(6\tau)^3}{\eta(\tau)^3\eta(3\tau)^3}\right)=\frac{6(2\tau+1)}{\pi}\eta(\tau)\eta(2\tau)\eta(3\tau)\eta(6\tau) \tag{4.44}$$

valid when the argument of p_4 is small and positive. This is the case for $\tau=-1/2+iy$ when $y>0$. Remarkably, the argument attains the value 1 at the quadratic irrationality $\tau=(\sqrt{-5/3}-1)/2$ (the 5/3rd singular value of the next section). As a consequence, the value $p_4(1)$ has a nice evaluation which is given in Theorem 4.5.1.

$\Diamond$

4.5 The density p_5

As shown in [BSW11], $W_5(s)$ has simple poles at $-2,-4,\ldots$, compare Figure 4.2(b). We write $r_{5,k}=\mathrm{Res}_{-2k-2}\,W_5$ for the residue of W_5 at $s=-2k-2$. A surprising bonus is an evaluation of $r_{5,0} = p_4(1) \approx 0.3299338011$, the residue at $s = -2$. This is because in general for $n \geqslant 4$, one has

$$\operatorname{Res}_{-2} W_{n+1} = p'_{n+1}(0) = p_n(1),$$

as follows from [BSW11, Prop. 1(b)]; here $p'_{n+1}(0)$ denotes the derivative from the right at zero.

Explicitly, using Theorem 4.4.9, we have,

$$r_{5,0} = p'_5(0) = \frac{2\sqrt{15}}{\pi^2} \operatorname{Re} {}_3F_2 \left({\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \atop \frac{5}{6}, \frac{7}{6}} \middle| \frac{125}{4} \right). \tag{4.45}$$

In fact, based on the modularity of p_4 discussed in Remark 4.4.11 we find:

Theorem 4.5.1.

$$r_{5,0} = \frac{1}{2\pi^2} \sqrt{\frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{5\Gamma(\frac{7}{15})\Gamma(\frac{11}{15})\Gamma(\frac{13}{15})\Gamma(\frac{14}{15})}}. \tag{4.46}$$

Proof. The value $\tau = (\sqrt{-5/3} - 1)/2$ in (4.44) gives the value $p_4(1) = r_{5,0}$. Applying the Chowla–Selberg formula [SC67, BB98] to evaluate the eta functions yields the claimed evaluation. $\square$

Using [BZ92, Table 4, (ii)], (4.46) may be simplified to

$$r_{5,0} = \frac{\sqrt{5}}{40} \frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{\pi^4} \tag{4.47}$$

$$= \frac{3\sqrt{5}}{\pi^3} \frac{\left(\sqrt{5}-1\right)}{2} K_{15}^2 = \frac{\sqrt{15}}{\pi^3} K_{5/3} K_{15}, \tag{4.48}$$

where K_{15} and $K_{5/3}$ are the complete elliptic integral at the 15th and 5/3rd singular values [BB98].

Remarkably, these evaluations appear to extend to $r_{5,1} \approx 0.006616730259$, the residue at $s = -4$. Resemblance to *the tiny nome of Bologna* [BBBG08] led us to discover — and then check to 400 places using (4.55) and (4.56) — that

$$r_{5,1} \stackrel{?}{=} \frac{13}{1800\sqrt{5}} \frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{\pi^4} - \frac{1}{\sqrt{5}} \frac{\Gamma(\frac{7}{15})\Gamma(\frac{11}{15})\Gamma(\frac{13}{15})\Gamma(\frac{14}{15})}{\pi^4}. \tag{4.49}$$

Using (4.47) this evaluation can be neatly restated as

$$r_{5,1} \stackrel{?}{=} \frac{13}{225} r_{5,0} - \frac{2}{5\pi^4} \frac{1}{r_{5,0}}. \tag{4.50}$$

We summarize our knowledge as follows:

Theorem 4.5.2. *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*

$$\begin{aligned} A_5 = {} & x^6(\theta+1)^4 - x^4(35\theta^4 + 42\theta^2 + 3) \\ & + x^2(259(\theta-1)^4 + 104(\theta-1)^2) - (15(\theta-3)(\theta-1))^2 \end{aligned} \tag{4.51}$$

and $\theta = xD_x$. Moreover, for small $x > 0$,

$$p_5(x) = \sum_{k=0}^{\infty} r_{5,k}\, x^{2k+1} \tag{4.52}$$

where

$$\begin{aligned} (15(2k+2)(2k+4))^2\, r_{5,k+2} = {} & \left(259(2k+2)^4 + 104(2k+2)^2\right) r_{5,k+1} \\ & - \left(35(2k+1)^4 + 42(2k+1)^2 + 3\right) r_{5,k} + (2k)^4 r_{5,k-1} \end{aligned} \tag{4.53}$$

with explicit initial values $r_{5,-1} = 0$ and $r_{5,0}$, $r_{5,1}$ given by (4.47) and (4.49) above.

Proof. First, the differential equation (4.51) is computed as was that for p_4, see (4.10). Next, as detailed in [BSW11, Ex. 3] the residues satisfy the recurrence relation (4.53) with the given initial values. Finally, proceeding as for (4.26), we deduce that (4.52) holds for small $x > 0$. $\square$

Numerically, the series (4.52) appears to converge for $|x| < 3$ which is in accordance with $\frac{1}{9}$ being a root of the characteristic polynomial of the recurrence (4.53); see also (4.12). The series (4.52) is depicted in Figure 4.3.

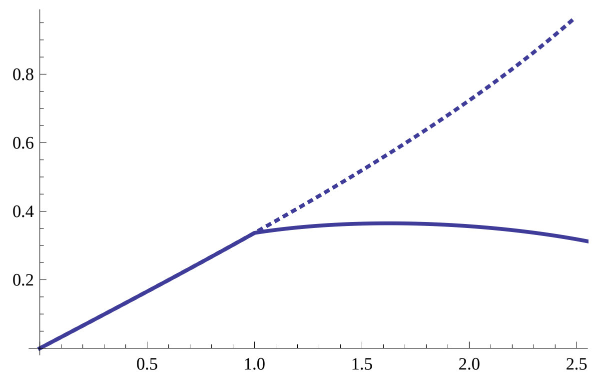


Figure 4.3: The series (4.52) (dotted) and p_5.

Since the poles of W_5 are simple, no logarithmic terms are involved in (4.52) as opposed to (4.26). In particular, by computing a few more residues from (4.53),

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

near 0 (with each coefficient given to six digits of precision only), explaining the strikingly straight shape of $p_5(x)$ on $[0, 1]$. This phenomenon was observed by Pearson [Pea06] 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, (4.5)] to give extremely close approximations to such simple forms as horizontal lines."

This conjecture was investigated in detail in [Fet63] wherein the nonlinearity was first rigorously established. This work and various more recent papers highlight the difficulty of computing the underlying Bessel integrals.

Remark 4.5.3. Recall from Example 4.4.3 that the asymptotic behaviour of p_n at zero is determined by the poles of the moments $W_n(s)$. To obtain information about the behaviour of $p_n(x)$ as $x \to n^-$, we consider the "reversed" densities $\tilde{p}_n(x) = p_n(n-x)$ and their moments $\tilde{W}_n(s)$. For non-negative integers k,

$$\tilde{W}_n(k) = \int_0^n x^k \tilde{p}_n(x)\,\mathrm{d}x = \int_0^n (n-x)^k p_n(x)\,\mathrm{d}x = \sum_{j=0}^{k} \binom{k}{j} (-1)^j n^{k-j} W_n(j)$$

On the other hand, we can find a recurrence satisfied by the $\tilde{W}_n(s)$ as follows: a differential equation for the densities $\tilde{p}_n(x)$ is obtained from Theorem 4.2.4 by a change of variables. The Mellin transform method as described in Example 4.2.3 then provides a recurrence for the moments $\tilde{W}_n(s)$. We next apply the same reasoning as in [BSW11] to obtain information about the pole structure of $\tilde{W}_n(s)$. It should be emphasized that this involves knowledge about initial conditions in term of explicit values of initial moments $W_n(2k)$.

For instance, in the case $n = 4$, we find that the moments $\tilde{W}_4(s)$ have simple poles at $-\frac{3}{2}, -\frac{5}{2}, -\frac{7}{2}, \ldots$ which predicts an expansion of $p_4(x)$ as given in Theorem 4.4.1.

For $n = 5$, we learn that $\tilde{W}_5(s)$ has simple poles at $s = -2, -3, -4, \ldots$. It then follows, as for (4.52), that $p_5(x) = \sum_{k=0}^{\infty} \tilde{r}_{5,k}\,(x-5)^{k+1}$ for $x \leqslant 5$ and close to 5. The $\tilde{r}_{5,k}$ are the residues of $\tilde{W}_5(s)$ at $s = -k-2$. $\Diamond$

4.6 Derivative evaluations of W_n

As illustrated by Theorem 4.4.4, 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. The residues may be obtained as a linear combination of the values of $W_n(s)$ and $W_n'(s)$.

Example 4.6.1 (Residues of W_n)**.** Using the functional equation for $W_3(s)$ and L'Hôpital's rule we find that the residue at $s = -2$ can be expressed as

$$\operatorname{Res}_{-2}(W_3) = \frac{8 + 12W_3'(0) - 4W_3'(2)}{9}. \tag{4.54}$$

This is a general principle and we likewise obtain for instance:

$$\operatorname{Res}_{-2}(W_5) = \frac{16 + 1140W_5'(0) - 804W_5'(2) + 64W_5'(4)}{225}, \tag{4.55}$$

$$\operatorname{Res}_{-4}(W_5) = \frac{26\operatorname{Res}_{-2}(W_5) - 16 - 20W_5'(0) + 4W_5'(2)}{225}. \tag{4.56}$$

In the presence of double poles, as for W_4,

$$\lim_{s\to-2}(s+2)^2 W_4(s) = \frac{3 + 4W_4'(0) - W_4'(2)}{8} \tag{4.57}$$

and for the residue:

$$\operatorname{Res}_{-2}(W_4) = \frac{9 + 18W_4'(0) - 3W_4'(2) + 4W_4''(0) - W_4''(2)}{16}. \tag{4.58}$$

Equations (4.57, 4.58) are used in Example 4.4.3 and each unknown is evaluated below. ◊

We are therefore interested in evaluations of the derivatives of W_n for even arguments.

Example 4.6.2 (Derivatives of W_3 and W_4)**.** Differentiating the double integral for $W_3(s)$ (4.7) under the integral sign, we have

$$W_3'(0) = \frac{1}{2}\int_0^1 \int_0^1 \log(4\sin(\pi y)\cos(2\pi x) + 3 - 2\cos(2\pi y))\,\mathrm{d}x\,\mathrm{d}y.$$

Then, using

$$\int_0^1 \log(a + b\cos(2\pi x))\,\mathrm{d}x = \log\left(\frac{1}{2}\left(a + \sqrt{a^2 - b^2}\right)\right) \text{ for } a > b > 0,$$

we deduce

$$W_3'(0) = \int_{1/6}^{5/6} \log(2\sin(\pi y))\,\mathrm{d}y = \frac{1}{\pi}\,\mathrm{Cl}\left(\frac{\pi}{3}\right), \tag{4.59}$$

where Cl denotes the *Clausen* function. Knowing as we do that the residue at $s = -2$ is $2/(\sqrt{3}\pi)$, we can thus also obtain from (4.54) that

$$W_3'(2) = 2 + \frac{3}{\pi}\,\mathrm{Cl}\left(\frac{\pi}{3}\right) - \frac{3\sqrt{3}}{2\pi}.$$

In like fashion,

$$\begin{aligned} W_4'(0) &= \frac{3}{8\pi^2}\int_0^\pi \int_0^\pi \log\left(3 + 2\,\cos x + 2\,\cos y + 2\,\cos(x-y)\right)\,\mathrm{d}x\,\mathrm{d}y \\ &= \frac{7}{2}\frac{\zeta(3)}{\pi^2}. \end{aligned} \tag{4.60}$$

The final equality will be shown in Example 4.6.6. Note that we may also write

$$W_3'(0) = \frac{1}{8\pi^2}\int_0^{2\pi} \int_0^{2\pi} \log(3 + 2\cos x + 2\cos y + 2\cos(x-y))\,\mathrm{d}x\,\mathrm{d}y.$$

The similarity between $W_3'(0)$ and $W_4'(0)$ is not coincidental, but comes from applying

$$\int_0^1 \log\left((a+\cos 2\pi x)^2 + (b+\sin 2\pi x)^2\right)\,\mathrm{d}x = \begin{cases} \log(a^2+b^2) & \text{if } a^2+b^2>1, \\ 0 & \text{otherwise} \end{cases}$$

to the triple integral of $W_4'(0)$. As this reduction breaks the symmetry, we cannot apply it to $W_5'(0)$ to get a similar integral. ♢

In general, differentiating the Bessel integral expression

$$W_n(s) = 2^{s+1-k}\frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})}\int_0^\infty x^{2k-s-1}\left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^k J_0^n(x)\,\mathrm{d}x, \tag{4.61}$$

obtained by David Broadhurst [Bro09] and discussed in [BSW11], under the integral sign gives

$$\begin{aligned} W_n'(0) &= n\int_0^\infty \left(\log\left(\frac{2}{x}\right)-\gamma\right) J_0^{n-1}(x)J_1(x)\,\mathrm{d}x \\ &= \log(2)-\gamma-n\int_0^\infty \log(x)J_0^{n-1}(x)J_1(x)\,\mathrm{d}x, \end{aligned} \tag{4.62}$$

where γ is the *Euler-Mascheroni* constant, and

$$W_n''(0) = n\int_0^\infty \left(\log\left(\frac{2}{x}\right)-\gamma\right)^2 J_0^{n-1}(x)J_1(x)\,\mathrm{d}x.$$

Likewise

$$W_n'(-1) = (\log(2)-\gamma)W_n(-1) - \int_0^\infty \log(x)J_0^n(x)\,\mathrm{d}x,$$

and

$$W_n'(1) = \int_0^\infty \frac{n}{x}J_0^{n-1}(x)J_1(x)\left(1-\gamma-\log(2x)\right)\,\mathrm{d}x.$$

Remark 4.6.3. We may therefore obtain many identities by comparing the above equations to known values. For instance,

$$3\int_0^\infty \log(x) J_0^2(x) J_1(x)\,\mathrm{d}x = \log(2) - \gamma - \frac{1}{\pi}\,\mathrm{Cl}\left(\frac{\pi}{3}\right).$$

$\Diamond$

Example 4.6.4 (Derivatives of W_5)**.** In the case $n = 5$,

$$W_5'(0) = 5\int_0^\infty \left(\log\left(\frac{2}{t}\right) - \gamma\right) J_0^4(t) J_1(t)\,\mathrm{d}t \approx 0.54441256$$

with similar but more elaborate formulae for $W_5'(2)$ and $W_5'(4)$. Observe that in general we also have

$$W_n'(0) = \log(2) - \gamma - \int_0^1 \left(J_0^n(x) - 1\right)\frac{\mathrm{d}x}{x} - \int_1^\infty J_0^n(x)\frac{\mathrm{d}x}{x}, \tag{4.63}$$

which is useful numerically. $\Diamond$

In fact, the hypergeometric representation of W_3 and W_4 first obtained in [Cra09] and recalled below also makes derivation of the derivatives of W_3 and W_4 possible.

Corollary 4.6.5 (Hypergeometric forms)**.** *For s not an odd integer, we have*

$$W_3(s) = \frac{1}{2^{2s+1}}\tan\left(\frac{\pi s}{2}\right)\binom{s}{\frac{s-1}{2}}^2 {}_3F_2\left(\left.{\frac{1}{2},\frac{1}{2},\frac{1}{2} \atop \frac{s+3}{2},\frac{s+3}{2}}\right|\frac{1}{4}\right) + \binom{s}{\frac{s}{2}}{}_3F_2\left(\left.{-\frac{s}{2},-\frac{s}{2},-\frac{s}{2} \atop 1,-\frac{s-1}{2}}\right|\frac{1}{4}\right), \tag{4.64}$$

and, if also $\mathrm{Re}\ s > -2$*, we have*

$$W_4(s) = \frac{1}{2^{2s}}\tan\left(\frac{\pi s}{2}\right)\binom{s}{\frac{s-1}{2}}^3 {}_4F_3\left(\left.{\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{s}{2}+1 \atop \frac{s+3}{2},\frac{s+3}{2},\frac{s+3}{2}}\right|1\right) + \binom{s}{\frac{s}{2}}{}_4F_3\left(\left.{\frac{1}{2},-\frac{s}{2},-\frac{s}{2},-\frac{s}{2} \atop 1,1,-\frac{s-1}{2}}\right|1\right). \tag{4.65}$$

Example 4.6.6 (Evaluation of $W_3'(0)$ and $W_4'(0)$)**.** If we write (4.64) or (4.65) as $W_n(s) = f_1(s)F_1(s) + f_2(s)F_2(s)$, where F_1, F_2 are the corresponding hypergeometric functions, then it can be readily verified that $f_1(0) = f_2'(0) = F_2'(0) = 0$. Thus, differentiating (4.64) by appealing to the product rule we get:

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

The last equality follows from setting $\theta = \pi/6$ in the identity

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

Likewise, differentiating (4.65) gives

$$W_4'(0) = \frac{4}{\pi^2} {}_4F_3\left(\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1 \\ \frac{3}{2}, \frac{3}{2}, \frac{3}{2}\end{matrix}\middle| 1\right) = \frac{7\zeta(3)}{2\pi^2}, \tag{4.66}$$

thus verifying (4.60). In this case the hypergeometric evaluation

$${}_4F_3\left(\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1 \\ \frac{3}{2}, \frac{3}{2}, \frac{3}{2}\end{matrix}\middle| 1\right) = \sum_{n=0}^{\infty} \frac{1}{(2n+1)^3} = \frac{7}{8}\zeta(3),$$

is elementary. $\diamond$

Differentiating (4.64) at $s = 2$ leads to the evaluation

$${}_3F_2\left(\begin{matrix}\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{2}, \frac{5}{2}\end{matrix}\middle| \frac{1}{4}\right) = \frac{27}{4}\left(\operatorname{Cl}\left(\frac{\pi}{3}\right) - \frac{\sqrt{3}}{2}\right),$$

while from (4.65) at $s = 2$ we obtain

$$W_4'(2) = 3 + \frac{14\zeta(3) - 12}{\pi^2}. \tag{4.67}$$

Thus we have enough information to evaluate (4.57) (with the answer $3/(2\pi^2)$).

Note that with two such starting values, all derivatives of $W_3(s)$ or $W_4(s)$ at even s may be computed recursively.

We also note here that the same technique yields

$$W_3''(0) = \frac{\pi^2}{12} - \frac{2}{\pi} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{4^{2n}} \frac{H_{n+1/2}}{(2n+1)^2} \tag{4.68}$$

$$= \frac{\pi^2}{12} + \frac{4\log(2)}{\pi} \operatorname{Cl}\left(\frac{\pi}{3}\right) - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{4^{2n}} \frac{\sum_{k=0}^{n} \frac{1}{2k+1}}{(2n+1)^2}, \tag{4.69}$$

and, quite remarkably,

$$W_4''(0) = \frac{\pi^2}{12} + \frac{7\zeta(3)\log(2)}{\pi^2} + \frac{4}{\pi^2} \sum_{n=0}^{\infty} \frac{H_n - 3H_{n+1/2}}{(2n+1)^3} \tag{4.70}$$

$$= \frac{24\mathrm{Li}_4\left(\frac{1}{2}\right) - 18\zeta(4) + 21\zeta(3)\log(2) - 6\zeta(2)\log^2(2) + \log^4(2)}{\pi^2},$$

where the very final evaluation is obtained from results in [BZB08, §5]. Here $\mathrm{Li}_4(1/2)$ is the *polylogarithm* of order 4, while $H_n := \gamma + \Psi(n+1)$ denotes the nth harmonic number, where Ψ is the *digamma* function. So for non-negative integers n, we have explicitly $H_n = \sum_{k=1}^{n} 1/k$, as before, and

$$H_{n+1/2} = 2\sum_{k=1}^{n+1} \frac{1}{2k-1} - 2\log(2).$$

An evaluation of $W_3''(0)$ in terms of polylogarithmic constants is given in [BS11a]. In particular, this gives an evaluation of the sum on the right-hand side of (4.68).

Finally, the corresponding sum for $W_4''(2)$ may be split into a telescoping part and a part involving $W_4''(0)$. Therefore, it can also be written as a linear combination of the constants used in (4.70). In summary, we have all the pieces to evaluate (4.58), obtaining the answer $9\log(2)/(2\pi^2)$.

4.6.1 Relations with Mahler measure

For a (Laurent) polynomial $f(x_1, \ldots, x_n)$, its *logarithmic Mahler measure*, see for instance [RVTV04], is defined as

$$m(f) = \int_0^1 \ldots \int_0^1 \log \left| f\left(e^{2\pi i t_1}, \ldots, e^{2\pi i t_n}\right) \right| \mathrm{d}t_1 \cdots \mathrm{d}t_n.$$

Recall that the sth moments of an n-step random walk are given by

$$W_n(s) = \int_0^1 \ldots \int_0^1 \left| \sum_{k=1}^n e^{2\pi i t_k} \right|^s \mathrm{d}t_1 \cdots \mathrm{d}t_n = \|x_1 + \ldots + x_n\|_s^s$$

where $\|\cdot\|_p$ denotes the p-norm over the unit n-torus, and hence

$$W_n'(0) = m(x_1 + \ldots + x_n) = m(1 + x_1 + \ldots + x_{n-1}).$$

Thus the derivative evaluations in the previous sections are also Mahler measure evaluations. In particular, we rediscovered

$$W_3'(0) = \frac{1}{\pi} \operatorname{Cl}\left(\frac{\pi}{3}\right) = L'(\chi_{-3}, -1) = m(1 + x_1 + x_2),$$

along with

$$W_4'(0) = \frac{7\zeta(3)}{2\pi^2} = m(1 + x_1 + x_2 + x_3)$$

which are both due to C. Smyth [RVTV04, (1.1) and (1.2)] with proofs first published in [Boy81, Appendix 1].

With this connection realized, we find the following conjectural expressions put forth by Rodriguez-Villegas, mentioned in different form in [Fin05],

$$W_5'(0) \stackrel{?}{=} \left(\frac{15}{4\pi^2}\right)^{5/2} \int_0^\infty \left\{\eta^3(e^{-3t})\eta^3(e^{-5t}) + \eta^3(e^{-t})\eta^3(e^{-15t})\right\} t^3 \,\mathrm{d}t \tag{4.71}$$

and

$$W_6'(0) \stackrel{?}{=} \left(\frac{3}{\pi^2}\right)^3 \int_0^\infty \eta^2(e^{-t})\eta^2(e^{-2t})\eta^2(e^{-3t})\eta^2(e^{-6t})\, t^4 \,\mathrm{d}t, \tag{4.72}$$

where η was defined in (4.42). We have confirmed numerically that the evaluation of $W_5'(0)$ in (4.71) holds to 600 places. Likewise, we have confirmed that (4.72) holds to 80 places. Details of these somewhat arduous confirmations are given in [BB11].

Differentiating the series expansion for $W_n(s)$ obtained in [BNSW11] term by term, we obtain

$$W_n'(0) = \log(n) - \sum_{m=1}^{\infty} \frac{1}{2m} \sum_{k=0}^{m} \binom{m}{k} \frac{(-1)^k W_n(2k)}{n^{2k}}. \tag{4.73}$$

On the other hand, from [RVTV04] we find the strikingly similar

$$W_n'(0) = \frac{1}{2}\log(n) - \frac{\gamma}{2} - \sum_{m=2}^{\infty} \frac{1}{2m} \sum_{k=0}^{m} \binom{m}{k} \frac{(-1)^k W_n(2k)}{k!\,n^k}. \tag{4.74}$$

Finally, we note that $W_n(s)$ itself is a special case of *zeta Mahler measure* as introduced recently in [Aka09].

4.7 New results on the moments W_n

From [BBBG08] equation (23), we have for $k > 0$ even,

$$W_3(k) = \frac{3^{k+3/2}}{\pi\, 2^k\, \Gamma(k/2+1)^2} \int_0^\infty t^{k+1} K_0(t)^2 I_0(t) \mathrm{d}t, \tag{4.75}$$

where $I_0(t), K_0(t)$ denote the *modified Bessel functions* of the first and second kind, respectively.

Similarly, [BBBG08] equation (55) states that for $k > 0$ even,

$$W_4(k) = \frac{4^{k+2}}{\pi^2\,\Gamma(k/2+1)^2}\int_0^\infty t^{k+1}K_0(t)^3 I_0(t)\mathrm{d}t. \tag{4.76}$$

Equation (4.75) can be formally reduced to a closed form as a ${}_3F_2$ (for instance by *Mathematica*). At $k = \pm 1$, the closed form agrees with $W_3(\pm 1)$. As both sides of (4.75) satisfy the same recursion ([BBBG08] equation (8)), we see that it in fact holds for all integers $k > -2$.

In the following we shall use Carlson's theorem ([Tit39]) which states:

Let f be analytic in the right half-plane $\mathrm{Re}\, z \geqslant 0$ *and of exponential type with the additional requirement that*

$$|f(z)| \leqslant Me^{d|z|}$$

for some $d < \pi$ on the imaginary axis $\mathrm{Re}\, z = 0$. *If $f(k) = 0$ for $k = 0, 1, 2, \ldots$ then $f(z) = 0$ identically.* We then have the following:

Lemma 4.7.1. *Equation (4.75) holds for all k with* $\mathrm{Re}\, k > -2$.

Proof. Both sides of (4.75) are of exponential type and agree when $k = 0, 1, 2, \ldots$. The standard estimate shows that the right-hand side grows like $e^{|y|\pi/2}$ on the imaginary axis. Therefore the conditions of Carlson's theorem are satisfied and the identity holds whenever the right-hand side converges. $\square$

Using the closed form given by the computer algebra system, we thus have:

Theorem 4.7.2 (Single hypergeometric for $W_3(s)$)**.** *For s not a negative integer < -1,*

$$W_3(s) = \frac{3^{s+3/2}}{2\pi}\frac{\Gamma(1+s/2)^2}{\Gamma(s+2)}\,{}_3F_2\left(\left.{\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2} \atop 1, \frac{s+3}{2}}\right|\frac{1}{4}\right). \tag{4.77}$$

Turning our attention to negative integers, we have for $k \geqslant 0$ an integer:

$$W_3(-2k-1) = \frac{4}{\pi^3}\left(\frac{2^k k!}{(2k)!}\right)^2 \int_0^\infty t^{2k} K_0(t)^3 \mathrm{d}t, \tag{4.78}$$

because the two sides satisfy the same recursion ([BBBG08, (8)]), and agree when $k = 0, 1$ ([BBBG08, (47) and (48)]).

Remark 4.7.3. Equation (4.78) however does not hold when k is not an integer. Also, combining (4.78) and (4.75) for $W_3(-1)$, we deduce

$$\int_0^\infty K_0(t)^2 I_0(t)\,\mathrm{d}t = \frac{2}{\sqrt{3}\pi}\int_0^\infty K_0(t)^3\,\mathrm{d}t = \frac{\pi^2}{2\sqrt{3}}\int_0^\infty J_0(t)^3\,\mathrm{d}t.$$

From (4.78), we experimentally determined a single hypergeometric for $W_3(s)$ at negative odd integers:

Lemma 4.7.4. *For $k \geqslant 0$ an integer,*

$$W_3(-2k-1) = \frac{\sqrt{3}\binom{2k}{k}^2}{2^{4k+1}3^{2k}}\,{}_3F_2\left(\left.{\frac{1}{2},\frac{1}{2},\frac{1}{2} \atop k+1, k+1}\right|\frac{1}{4}\right).$$

Proof. It is easy to check that both sides agree at $k = 0, 1$. Therefore we need only to show that they satisfy the same recursion. The recursion for the left-hand side implies a contiguous relation for the right-hand side, which can be verified by extracting the summand and applying Gosper's algorithm ([PWZ96]). $\square$

The integral in (4.78) shows that $W_3(-2k-1)$ decays to 0 rapidly – very roughly like 9^{-k} as $k \to \infty$ – and so is never 0 when k is an integer.

To show that (4.76) holds for more general k required more work. Using Nicholson's integral representation in [Wat41],

$$I_0(t)K_0(t) = \frac{2}{\pi}\int_0^{\pi/2} K_0(2t\sin a)\,\mathrm{d}a,$$

the integral in (4.76) simplifies to

$$\frac{2}{\pi}\int_0^{\pi/2}\int_0^{\infty} t^{k+1}K_0(t)^2K_0(2t\sin a)\,\mathrm{d}t\mathrm{d}a. \tag{4.79}$$

The inner integral in (4.79) simplifies in terms of a *Meijer G-function*; *Mathematica* is able to produce

$$\frac{\sqrt{\pi}}{8\sin^{k+2}a}\,G_{3,3}^{3,2}\left(\begin{matrix}-\frac{1}{2},-\frac{1}{2},\frac{1}{2}\\ 0,0,0\end{matrix}\middle|\frac{1}{\sin^2 a}\right),$$

which transforms to

$$\frac{\sqrt{\pi}}{8\sin^{k+2}a}\,G_{3,3}^{2,3}\left(\begin{matrix}1,1,1\\ \frac{3}{2},\frac{3}{2},\frac{1}{2}\end{matrix}\middle|\sin^2 a\right).$$

Let $t=\sin^2 a$ in the above, so the outer integral in (4.79) transforms to

$$\frac{\sqrt{\pi}}{16}\int_0^1 t^{-\frac{k+3}{2}}(1-t)^{-\frac{1}{2}}\,G_{3,3}^{2,3}\left(\begin{matrix}1,1,1\\ \frac{3}{2},\frac{3}{2},\frac{1}{2}\end{matrix}\middle|t\right)\mathrm{d}t. \tag{4.80}$$

We can resolve this integral by applying the Euler-type integral

$$\int_0^1 t^{-a}(1-t)^{a-b-1}\,G_{p,q}^{m,n}\left(\begin{matrix}\mathbf{c}\\ \mathbf{d}\end{matrix}\middle|zt\right)\mathrm{d}t=\Gamma(a-b)\,G_{p+1,q+1}^{m,n+1}\left(\begin{matrix}a,\mathbf{c}\\ \mathbf{d},b\end{matrix}\middle|z\right). \tag{4.81}$$

Indeed, when $k=-1$, the application of (4.81) recovers the Meijer G representation of $W_4(-1)$ ([BSW11]); that is, (4.76) holds for $k=-1$.

When $k=1$, the resulting Meijer G-function is

$$G_{4,4}^{2,4}\left(\begin{matrix}2,1,1,1\\ \frac{3}{2},\frac{3}{2},\frac{1}{2},\frac{3}{2}\end{matrix}\middle|1\right),$$

to which we apply Nesterenko's theorem ([Nes03]), deducing a triple integral (up to a constant factor) for it:

$$\int_0^1\int_0^1\int_0^1\sqrt{\frac{x(1-x)z}{y(1-y)(1-z)(1-x(1-yz))^3}}\,\mathrm{d}x\mathrm{d}y\mathrm{d}z.$$

We can reduce the triple integral to a single integral,

$$\int_0^1 \frac{8E'(t)\big((1+t^2)K'(t) - 2E'(t)\big)}{(1-t^2)^2}\,\mathrm{d}t.$$

Now applying the change of variable $t \mapsto (1-t)/(1+t)$, followed by quadratic transformations for K and E, we finally get

$$\int_0^1 \frac{4(1+t)}{t^2} E\left(\frac{2\sqrt{t}}{1+t}\right)\big(K(t) - E(t)\big)\,\mathrm{d}t,$$

which is, indeed, (a correct constant multiple times) the expression for $W_4(1)$ which follows from Section 3.1 in [BSW11].

We finally observe that both sides of (4.76) satisfy the same recursion ([BBBG08] equation (9)), hence they agree for $k = 0, 1, 2, \ldots$. Carlson's theorem applies with the same growth on the imaginary axis as in (4.75) and we have proven the following:

Lemma 4.7.5. *Equation (4.76) holds for all k with $\operatorname{Re} k > -2$.*

Theorem 4.7.6 (Alternative Meijer G representation for $W_4(s)$)**.** *For all s,*

$$W_4(s) = \frac{2^{2s+1}}{\pi^2\,\Gamma(\frac{1}{2}(s+2))^2}\, G^{2,4}_{4,4}\left(\begin{matrix}1, 1, 1, \frac{s+3}{2} \\ \frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2}, \frac{1}{2}\end{matrix}\,\middle|\, 1\right). \tag{4.82}$$

Proof. Apply (4.81) to (4.80) for general k, and equality holds by Lemma 4.7.5. □

Note that Lemma 4.7.5 combined with the known formula for $W_4(-1)$ in [BSW11] gives

$$\frac{4}{\pi^3}\int_0^\infty K_0(t)^3 I_0(t)\,\mathrm{d}t = \int_0^\infty J_0(t)^4\,\mathrm{d}t.$$

Armed with the knowledge of Lemma 4.7.5, we may now resolve a very special but central case (corresponding to $n = 2$) of Conjecture 1 in [BSW11].

Theorem 4.7.7. *For integer s,*

$$W_4(s) = \sum_{j=0}^{\infty} \binom{s/2}{j}^2 W_3(s-2j). \tag{4.83}$$

Proof. In [BNSW11] it is shown that both sides satisfy the same three term recurrence, and agree when s is even. Therefore, we only need to show that the identity holds for two consecutive odd values of s.

For $s = -1$, the right-hand side of (4.83) is

$$\sum_{j=0}^{\infty} \binom{-1/2}{j}^2 W_3(-1-2j) = \sum_{j=0}^{\infty} \frac{2^{2-2j}}{\pi^3 j!^2} \int_0^{\infty} t^{2j} K_0(t)^3 \,\mathrm{d}t$$

upon using (4.78), and after interchanging summation and integration (which is justified as all terms are positive), this reduces to

$$\frac{4}{\pi^3} \int_0^{\infty} K_0(t)^3 I_0(t) \,\mathrm{d}t,$$

which is the value for $W_4(-1)$ by Lemma 4.7.5.

We note that the recursion for $W_4(s)$ gives the pleasing reflection property

$$W_4(-2k-1)\, 2^{6k} = W_4(2k-1).$$

In particular, $W_4(-3) = \frac{1}{64} W_4(1)$. Now computing the right-hand side of (4.83) at $s = -3$, and interchanging summation and integration as before, we obtain

$$\sum_{j=0}^{\infty} \binom{-3/2}{j}^2 W_3(-3-2j) = \frac{4}{\pi^3} \int_0^{\infty} t^2 K_0(t)^3 I_0(t) \,\mathrm{d}t = \frac{1}{64} W_4(1) = W_4(-3).$$

Therefore (4.83) holds when $s = -1, -3$, and thus holds for all integer s. $\square$

4.8 Appendix: A family of combinatorial identities

DON ZAGIER[1]

The "collateral result" of Djakov and Mityagin, [DM04, DM07], is the pair of identities

$$\sum_{\substack{-m<i_1<\cdots<i_k<m \\ i_2-i_1,\dots,i_k-i_{k-1}\geqslant 2}} \prod_{s=1}^{k}(m^2-i_s^2) = \sigma_k(1^2,3^2,\dots,(2m-1)^2)\,,$$

$$\sum_{\substack{1-m<i_1<\cdots<i_k<m \\ i_2-i_1,\dots,i_k-i_{k-1}\geqslant 2}} \prod_{s=1}^{k}(m-i_s)(m+i_s-1) = \sigma_k(2^2,4^2,\dots,(2m-2)^2)\,,$$

where m and k are integers with $m \geqslant k \geqslant 0$ and σ_k denotes the kth elementary symmetric function. By setting $j_s = i_s + m$ in the first sum and $j_s = i_s + m - 1$ in the second, we can rewrite these formulas more uniformly as[2]

$$F_{M,k}(M) = \begin{cases} \sigma_k(1^2,3^2,\dots,(M-1)^2) & \text{if } M \text{ is even,} \\ \sigma_k(2^2,4^2,\dots,(M-1)^2) & \text{if } M \text{ is odd,} \end{cases} \tag{4.84}$$

where $F_{M,k}(X)$ is the polynomial in X (non-zero only if $M \geqslant 2k \geqslant 0$) defined by

$$F_{M,k}(X) = \sum_{\substack{0<j_1<\cdots<j_k<M \\ j_2-j_1,\dots,j_k-j_{k-1}\geqslant 2}} \prod_{s=1}^{k} j_s(X-j_s)\,. \tag{4.85}$$

[1]The original note is unchanged.
[2]Note that (4.84) is precisely Theorem 4.2.7.

The advantage of introducing the free variable X in (4.85) is that the functions $F_{M,k}(X)$ satisfy the recursion

$$F_{M+1,k+1}(X) - F_{M,k+1}(X) = M\,(X-M)\,F_{M-1,k}(X), \tag{4.86}$$

because the only paths that are counted on the left are those with $0 < j_1 < \cdots < j_k < j_{k+1} = M$.

It is also advantageous to introduce the polynomial generating function

$$\Phi_M = \Phi_M(X,u) = \sum_{0 \leqslant k \leqslant M/2} (-1)^k\, F_{M,k}(X)\, u^{M-2k}\,,$$

the first examples being

$$\Phi_0 = 1\,, \qquad \Phi_1 = u\,, \qquad \Phi_2 = u^2 - (X-1)\,, \qquad \Phi_3 = u^3 - (3X-5)u\,,$$
$$\Phi_4 = u^4 - (6X-14)u^2 + (3X^2 - 12X + 9)\,,$$
$$\Phi_5 = u^5 - (10X-30)u^3 + (15X^2 - 80X + 89)\,,$$
$$\Phi_6 = u^6 - (15X-55)u^4 + (45X^2 - 300X + 439)u^2 - (15X^3 - 135X^2 + 345X - 225)\,.$$

In terms of this generating function, the recursion (4.86) becomes

$$\Phi_{M+1} = u\,\Phi_M - M(X-M)\,\Phi_{M-1} \tag{4.87}$$

and the identity (4.84) to be proved can be written succinctly as

$$\Phi_M(M,u) = \prod_{\substack{|\lambda|<M \\ \lambda \not\equiv M \pmod 2}} (u-\lambda)\,. \tag{4.88}$$

Denote by $P_M(u)$ the polynomial on the right-hand side of (4.88). Looking for other pairs (M,X) where $\Phi_M(X,u)$ has many integer roots, we find experimentally that this happens whenever $M - X$ is a non-negative integer, and studying the data more closely we are to conjecture the two formulas

$$\Phi_M(M-n,u) = \frac{1}{2^n}\sum_{j=0}^{n}\binom{n}{j}P_M(u-n+2j) \qquad (M,\,n\geqslant 0) \tag{4.89}$$

(a generalization of (4.88)) and

$$\Phi_{M+n}(M,u) = \Phi_M(M,u)\,\Phi_n(-M,u) \qquad (M,\,n\geqslant 0)\,. \tag{4.90}$$

Formula (4.90) is easy to prove, since it holds for $n = 0$ trivially and for $n = 1$ by (4.87) and since both sides satisfy the recursion $y_{n+1} = u\,y_n + n(M+n)\,y_{n-1}$ for $n = 1, 2, \dots$ by (4.87). On the other hand, combining (4.88), (4.89) and (4.90) leads to the conjectural formula

$$\Phi_n(-M,u) = \frac{1}{2^n}\sum_{j=0}^{n}\binom{n}{j}\frac{P_{M+n}(u-n+2j)}{P_n(u)} = n!\sum_{j=0}^{n}(-1)^j\binom{\frac{-u-M-1}{2}}{j}\binom{\frac{u-M-1}{2}}{n-j}$$

or, renaming the variables,

$$\frac{1}{M!}\,\Phi_M(x+y+1,y-x) = \sum_{j=0}^{M}(-1)^j\binom{x}{j}\binom{y}{M-j}\,. \tag{4.91}$$

To prove this, we see by (4.87) that, denoting by $G_M = G_M(x,y)$ the expression on the right, it suffices to prove the recursion $(M+1)G_{M+1} = (y-x)G_M + (M-x-y-1)G_{M-1}$. This is an easy binomial coefficient identity, but once again it is easier to work with generating functions: the sum

$$\mathcal{G}(x,y;T) := \sum_{M=0}^{\infty} G_M(x,y)\,T^m = (1-T)^x\,(1+T)^y \tag{4.92}$$

satisfies the differential equation

$$\frac{1}{\mathcal{G}}\frac{\partial \mathcal{G}}{\partial T} = \frac{y}{1+T} - \frac{x}{1-T}$$

or

$$\frac{\partial \mathcal{G}}{\partial T} = (y-x)\,\mathcal{G} + \left(T\frac{\partial}{\partial T} - x - y\right)\mathcal{G},$$

and this is equivalent to the desired recursion.

We can now complete the proof of (4.84). Rewriting (4.92) in the form

$$\frac{1}{M!}\,\Phi_M(X,u) = \mathrm{coeff}_{T^M}\left((1-T)^{\frac{X-u-1}{2}}\,(1+T)^{\frac{X+u-1}{2}}\right)\,,$$

we find that, for $1 \leqslant j \leqslant M$,

$$\frac{1}{M!}\,\Phi_M(M, M+1-2j) = \mathrm{coeff}_{T^M}\left((1-T)^{j-1}\,(1+T)^{M-j}\right) = 0$$

and hence that the polynomial on the left-hand side of (4.88) is divisible by the polynomial on the right, which completes the proof since both are monic of degree M in u.

Chapter 5

Special values of generalized log-sine integrals

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[BS11c] *Special values of generalized log-sine integrals*
(with Jonathan M. Borwein)
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Abstract We study generalized log-sine integrals at special values. At π and multiples thereof explicit evaluations are obtained in terms of Nielsen polylogarithms at ± 1. For general arguments we present algorithmic evaluations involving Nielsen polylogarithms at related arguments. In particular, we consider log-sine integrals at $\pi/3$ which evaluate in terms of polylogarithms at the sixth root of unity. An implementation of our results for the computer algebra systems *Mathematica* and SAGE is provided.

5.1 Introduction

For $n = 1, 2, \dots$ and $k \geqslant 0$, we consider the (generalized) *log-sine integrals* defined by

$$\mathrm{Ls}_n^{(k)}(\sigma) := -\int_0^\sigma \theta^k \log^{n-1-k}\left|2\sin\frac{\theta}{2}\right| \mathrm{d}\theta. \tag{5.1}$$

The modulus is not needed for $0 \leqslant \sigma \leqslant 2\pi$. For $k = 0$ these are the (basic) log-sine integrals $\mathrm{Ls}_n(\sigma) := \mathrm{Ls}_n^{(0)}(\sigma)$. Various log-sine integral evaluations may be found in [Lew81, §7.6 & §7.9].

In this paper, we will be concerned with evaluations of the log-sine integrals $\mathrm{Ls}_n^{(k)}(\sigma)$ for special values of σ. Such evaluations are useful for physics [KS05]: log-sine integrals appeared for instance in recent work on the ε-expansion of various Feynman diagrams in the calculation of higher terms in the ε-expansion, [DK00, KV00, DK01, Dav00, Kal05]. Of particular importance are the log-sine integrals at the special values $\pi/3$, $\pi/2$, $2\pi/3$, π. The log-sine integrals also appear in many settings in number theory and analysis: classes of inverse binomial sums can be expressed in terms of generalized log-sine integrals, [DK04, BBK01].

In Section 5.2 we focus on evaluations of log-sine and related integrals at π. General arguments are considered in Section 5.4 with a focus on the case $\pi/3$ in Section 5.4.1. Imaginary arguments are briefly discussed in 5.4.2. The results obtained are suitable for implementation in a computer algebra system. Such an implementation is provided for *Mathematica* and SAGE, and is described in Section 5.6. This complements existing packages such as `lsjk` [KS05] for numerical evaluations of log-sine integrals or `HPL` [Mai06] as well as [VW05] for working with multiple polylogarithms.

Further motivation for such evaluations was sparked by our recent study [BS11a] of certain *multiple Mahler measures*. For k functions (typically Laurent polynomials) in n variables the multiple Mahler measure $\mu(P_1, P_2, \dots, P_k)$, introduced in [KLO08], is defined by

$$\int_0^1 \cdots \int_0^1 \prod_{j=1}^{k} \log \left| P_j \left(e^{2\pi i t_1}, \ldots, e^{2\pi i t_n} \right) \right| \mathrm{d}t_1 \mathrm{d}t_2 \ldots \mathrm{d}t_n.$$

When $P = P_1 = P_2 = \cdots = P_k$ this devolves to a *higher Mahler measure*, $\mu_k(P)$, as introduced and examined in [KLO08]. When $k = 1$ both reduce to the standard (logarithmic) *Mahler measure* [Boy81].

The multiple Mahler measure

$$\mu_k(1 + x + y_*) := \mu(1 + x + y_1, 1 + x + y_2, \ldots, 1 + x + y_k) \tag{5.2}$$

was studied by Sasaki [Sas10, Lemma 1] who provided an evaluation of $\mu_2(1+x+y_*)$. It was observed in [BS11a] that

$$\mu_k(1 + x + y_*) = \frac{1}{\pi} \operatorname{Ls}_{k+1}\left(\frac{\pi}{3}\right) - \frac{1}{\pi} \operatorname{Ls}_{k+1}(\pi). \tag{5.3}$$

Many other Mahler measures studied in [BS11a, BBSW12] were shown to have evaluations involving generalized log-sine integrals at π and $\pi/3$ as well.

To our knowledge, this is the most exacting such study undertaken — perhaps because it would be quite impossible without modern computational tools and absent a use of the quite recent understanding of multiple polylogarithms and multiple zeta values [BBBL01].

5.2 Evaluations at π

5.2.1 Basic log-sine integrals at π

The exponential generating function, [Lew58, Lew81],

$$-\frac{1}{\pi}\sum_{m=0}^{\infty}\mathrm{Ls}_{m+1}(\pi)\,\frac{\lambda^m}{m!}=\frac{\Gamma(1+\lambda)}{\Gamma^2\left(1+\frac{\lambda}{2}\right)}=\binom{\lambda}{\frac{\lambda}{2}} \tag{5.4}$$

is well-known and implies the recurrence

$$\begin{aligned}\frac{(-1)^n}{n!}\,\mathrm{Ls}_{n+2}(\pi)&=\pi\,\alpha(n+1)\\&\quad+\sum_{k=1}^{n-2}\frac{(-1)^k}{(k+1)!}\,\alpha(n-k)\,\mathrm{Ls}_{k+2}(\pi)\,,\end{aligned} \tag{5.5}$$

where $\alpha(m)=(1-2^{1-m})\zeta(m)$.

Example 5.2.1. (Values of $\mathrm{Ls}_n(\pi)$) We have $\mathrm{Ls}_2(\pi)=0$ and

$$\begin{aligned}-\mathrm{Ls}_3(\pi)&=\frac{1}{12}\,\pi^3\\ \mathrm{Ls}_4(\pi)&=\frac{3}{2}\pi\,\zeta(3)\\ -\mathrm{Ls}_5(\pi)&=\frac{19}{240}\,\pi^5\\ \mathrm{Ls}_6(\pi)&=\frac{45}{2}\,\pi\,\zeta(5)+\frac{5}{4}\,\pi^3\zeta(3)\\ -\mathrm{Ls}_7(\pi)&=\frac{275}{1344}\,\pi^7+\frac{45}{2}\,\pi\,\zeta(3)^2\\ \mathrm{Ls}_8(\pi)&=\frac{2835}{4}\,\pi\,\zeta(7)+\frac{315}{8}\,\pi^3\zeta(5)+\frac{133}{32}\,\pi^5\zeta(3),\end{aligned}$$

and so forth. The fact that each integral is a multivariable rational polynomial in π and zeta values follows directly from the recursion (5.5). Alternatively, these values may be conveniently obtained from (5.4) by a computer algebra system. For instance, in *Mathematica* the code

```
FullSimplify[D[-Binomial[x,x/2], {x,6}] /.x->0]
```

produces the above evaluation of $\mathrm{Ls}_6(\pi)$. $\diamondsuit$

5.2.2 The log-sine-cosine integrals

The log-sine-cosine integrals

$$\mathrm{Lsc}_{m,n}(\sigma) := -\int_0^\sigma \log^{m-1}\left|2\sin\frac{\theta}{2}\right| \log^{n-1}\left|2\cos\frac{\theta}{2}\right| \mathrm{d}\theta \tag{5.6}$$

appear in physical applications as well, see for instance [DK01, Kal05]. They have also been considered by Lewin, [Lew58, Lew81], and he demonstrates how their values at $\sigma = \pi$ may be obtained much the same as those of the log-sine integrals in Section 5.2.1. As observed in [BBSW12], Lewin's result can be put in the form

$$\begin{aligned} -\frac{1}{\pi}\sum_{m,n=0}^{\infty} \mathrm{Lsc}_{m+1,n+1}(\pi)\frac{x^m}{m!}\frac{y^n}{n!} &= \frac{2^{x+y}}{\pi}\frac{\Gamma\left(\frac{1+x}{2}\right)\Gamma\left(\frac{1+y}{2}\right)}{\Gamma\left(1+\frac{x+y}{2}\right)} \\ &= \binom{x}{x/2}\binom{y}{y/2}\frac{\Gamma\left(1+\frac{x}{2}\right)\Gamma\left(1+\frac{y}{2}\right)}{\Gamma\left(1+\frac{x+y}{2}\right)}. \end{aligned} \tag{5.7}$$

The last form makes it clear that this is an extension of (5.4).

The notation Lsc has been introduced in [DK01] where evaluations for other values of σ and low weight can be found.

5.2.3 Log-sine integrals at π

As Lewin [Lew81, §7.9] sketches, at least for small values of n and k, the generalized log-sine integrals $\mathrm{Ls}_n^{(k)}(\pi)$ have closed forms involving zeta values and Kummer-type constants such as $\mathrm{Li}_4(1/2)$. This will be made more precise in Remark 5.2.8.

Our analysis starts with the generating function identity

$$
\begin{aligned}
&-\sum_{n,k\geqslant 0} \mathrm{Ls}_{n+k+1}^{(k)}(\pi)\,\frac{\lambda^n}{n!}\frac{(i\mu)^k}{k!} = \int_0^\pi \left(2\sin\frac{\theta}{2}\right)^\lambda \mathrm{e}^{i\mu\theta}\,\mathrm{d}\theta \\
&= i\mathrm{e}^{i\pi\frac{\lambda}{2}}\,B_1\left(\mu-\tfrac{\lambda}{2},1+\lambda\right) - i\mathrm{e}^{i\pi\mu}B_{1/2}\left(\mu-\tfrac{\lambda}{2},-\mu-\tfrac{\lambda}{2}\right) \qquad (5.8)
\end{aligned}
$$

given in [Lew81]. Here B_x is the *incomplete Beta* function:

$$B_x(a,b) = \int_0^x t^{a-1}(1-t)^{b-1}\,\mathrm{d}t.$$

We shall show that with care — because of the singularities at zero — (5.8) can be differentiated as needed as suggested by Lewin.

Using the identities, valid for $a,b>0$ and $0<x<1$,

$$
\begin{aligned}
B_x(a,b) &= \frac{x^a(1-x)^{b-1}}{a}\,{}_2F_1\left(\begin{matrix}1-b,1\\ a+1\end{matrix}\middle|\frac{x}{x-1}\right) \\
&= \frac{x^a(1-x)^{b}}{a}\,{}_2F_1\left(\begin{matrix}a+b,1\\ a+1\end{matrix}\middle|x\right),
\end{aligned}
$$

found for instance in [OLBC10, §8.17(ii)], the generating function (5.8) can be rewritten as

$$i\mathrm{e}^{i\pi\frac{\lambda}{2}}\left(B_1\left(\mu-\frac{\lambda}{2},1+\lambda\right) - B_{-1}\left(\mu-\frac{\lambda}{2},1+\lambda\right)\right).$$

Upon expanding this we obtain the following computationally more accessible generating function for $\mathrm{Ls}_{n+k+1}^{(k)}(\pi)$:

Theorem 5.2.2. *For* $2|\mu| < \lambda < 1$ *we have*

$$\begin{aligned} -\sum_{n,k\geqslant 0} \mathrm{Ls}^{(k)}_{n+k+1}(\pi)\,\frac{\lambda^n}{n!}\frac{(i\mu)^k}{k!} \\ = i\sum_{n\geqslant 0}\binom{\lambda}{n}\frac{(-1)^n \mathrm{e}^{i\pi\frac{\lambda}{2}} - \mathrm{e}^{i\pi\mu}}{\mu - \frac{\lambda}{2} + n}. \end{aligned} \tag{5.9}$$

We now show how the log-sine integrals $\mathrm{Ls}^{(k)}_n(\pi)$ can quite comfortably be extracted from (5.9) by differentiating its right-hand side. The case $n = 0$ is covered by:

Proposition 5.2.3. *We have*

$$\frac{\mathrm{d}^k}{\mathrm{d}\mu^k}\frac{\mathrm{d}^m}{\mathrm{d}\lambda^m} i\frac{\mathrm{e}^{i\pi\frac{\lambda}{2}} - \mathrm{e}^{i\pi\mu}}{\mu - \frac{\lambda}{2}}\bigg|_{\substack{\lambda=0\\ \mu=0}} = \frac{\pi}{2^m}(i\pi)^{m+k} B(m+1, k+1).$$

Proof. This may be deduced from

$$\begin{aligned} \frac{\mathrm{e}^x - \mathrm{e}^y}{x - y} &= \sum_{m,k\geqslant 0} \frac{x^m y^k}{(k+m+1)!} \\ &= \sum_{m,k\geqslant 0} B(m+1, k+1)\frac{x^m}{m!}\frac{y^k}{k!} \end{aligned}$$

upon setting $x = i\pi\lambda/2$ and $y = i\pi\mu$. □

The next proposition is most helpful in differentiation of the right-hand side of (5.9) for $n \geqslant 1$, Here, we denote a *multiple harmonic number* by

$$H^{[\alpha]}_{n-1} := \sum_{n>i_1>i_2>\ldots>i_\alpha} \frac{1}{i_1 i_2 \cdots i_\alpha}. \tag{5.10}$$

If $\alpha = 0$ we set $H^{[0]}_{n-1} := 1$.

Proposition 5.2.4. *For $n \geqslant 1$*

$$\frac{(-1)^\alpha}{\alpha!}\left(\frac{\mathrm{d}}{\mathrm{d}\lambda}\right)^\alpha \binom{\lambda}{n}\bigg|_{\lambda=0} = \frac{(-1)^n}{n} H_{n-1}^{[\alpha-1]}. \tag{5.11}$$

Note that, for $\alpha \geqslant 0$,

$$\sum_{n\geqslant 0} \frac{(\pm 1)^n}{n^\beta} H_{n-1}^{[\alpha]} = \mathrm{Li}_{\beta,\{1\}^\alpha}(\pm 1)$$

which shows that the evaluation of the log-sine integrals will involve Nielsen polylogarithms at ± 1, that is polylogarithms of the type $\mathrm{Li}_{a,\{1\}^b}(\pm 1)$.

Using the Leibniz rule coupled with Proposition 5.2.4 to differentiate (5.9) for $n \geqslant 1$ and Proposition 5.2.3 in the case $n = 0$, it is possible to explicitly write $\mathrm{Ls}_n^{(k)}(\pi)$ as a finite sum of Nielsen polylogarithms with coefficients only being rational multiples of powers of π. The process is now exemplified for $\mathrm{Ls}_4^{(2)}(\pi)$ and $\mathrm{Ls}_5^{(1)}(\pi)$.

Example 5.2.5. ($\mathrm{Ls}_4^{(2)}(\pi)$) To find $\mathrm{Ls}_4^{(2)}(\pi)$ we differentiate (5.9) once with respect to λ and twice with respect to μ. To simplify computation, we exploit the fact that the result will be real which allows us to neglect imaginary parts:

$$\begin{aligned} -\mathrm{Ls}_4^{(2)}(\pi) &= \frac{\mathrm{d}^2}{\mathrm{d}\mu^2}\frac{\mathrm{d}}{\mathrm{d}\lambda} i \sum_{n\geqslant 0}\binom{\lambda}{n}\frac{(-1)^n \mathrm{e}^{i\pi\frac{\lambda}{2}} - \mathrm{e}^{i\pi\mu}}{\mu - \frac{\lambda}{2} + n}\bigg|_{\lambda=\mu=0} \\ &= 2\pi \sum_{n\geqslant 1}\frac{(-1)^{n+1}}{n^3} = \frac{3}{2}\pi\zeta(3). \end{aligned}$$

In the second step we were able to drop the term corresponding to $n = 0$ because its contribution $-i\pi^4/24$ is purely imaginary as follows a priori from Proposition 5.2.4.

$\Diamond$

Example 5.2.6. ($\mathrm{Ls}_5^{(1)}(\pi)$) Similarly, setting

$$\mathrm{Li}^{\pm}_{a_1,\ldots,a_n} := \mathrm{Li}_{a_1,\ldots,a_n}(1) - \mathrm{Li}_{a_1,\ldots,a_n}(-1)$$

we obtain $\mathrm{Ls}_5^{(1)}(\pi)$ as

$$\begin{aligned}
-\mathrm{Ls}_5^{(1)}(\pi) &= \frac{3}{4}\sum_{n\geqslant 1}\frac{8(1-(-1)^n)}{n^4}\left(nH_{n-1}^{[2]}-H_{n-1}\right)\\
&\qquad+\frac{6(1-(-1)^n)}{n^5}-\frac{\pi^2}{n^3}\\
&= 6\,\mathrm{Li}_{3,1,1}^{\pm}-6\,\mathrm{Li}_{4,1}^{\pm}+\frac{9}{2}\,\mathrm{Li}_5^{\pm}-\frac{3}{4}\pi^2\zeta(3)\\
&= -6\,\mathrm{Li}_{3,1,1}(-1)+\frac{105}{32}\zeta(5)-\frac{1}{4}\pi^2\zeta(3).
\end{aligned}$$

The last form is what is automatically produced by our program, see Example 5.6.1, and is obtained from the previous expression by reducing the polylogarithms as discussed in Section 5.5. $\diamondsuit$

The next example hints at the rapidly growing complexity of these integrals, especially when compared to the evaluations given in Examples 5.2.5 and 5.2.6.

Example 5.2.7. ($\mathrm{Ls}_6^{(1)}(\pi)$) Proceeding as before we find

$$\begin{aligned}
-\mathrm{Ls}_6^{(1)}(\pi) &= -24\,\mathrm{Li}_{3,1,1,1}^{\pm}+24\,\mathrm{Li}_{4,1,1}^{\pm}-18\,\mathrm{Li}_{5,1}^{\pm}+12\,\mathrm{Li}_6^{\pm}\\
&\qquad+3\pi^2\zeta(3,1)-3\pi^2\zeta(4)+\frac{\pi^6}{480}\\
&= 24\,\mathrm{Li}_{3,1,1,1}(-1)-18\,\mathrm{Li}_{5,1}(-1)\\
&\qquad+3\zeta(3)^2-\frac{3}{1120}\pi^6.
\end{aligned}\tag{5.12}$$

In the first equality, the term $\pi^6/480$ is the one corresponding to $n=0$ in (5.9) obtained from Proposition 5.2.3. The second form is again the automatically reduced output of our program. $\diamondsuit$

Remark 5.2.8. From the form of (5.9) and (5.11) we find that the log-sine integrals $\mathrm{Ls}_n^{(k)}(\pi)$ can be expressed in terms of π and Nielsen polylogarithms at ± 1. Using the duality results in [BBBL01, §6.3, and Example 2.4] the polylogarithms at -1 may be explicitly reexpressed as multiple polylogarithms at $1/2$. Some examples are given in [BS11a].

Particular cases of Theorem 5.2.2 have been considered in [KS05] where explicit formulae are given for $\mathrm{Ls}_n^{(k)}(\pi)$ where $k = 0, 1, 2$. $\Diamond$

5.2.4 Log-sine integrals at 2π

As observed by Lewin [Lew81, 7.9.8], log-sine integrals at 2π are expressible in terms of zeta values only. If we proceed as in the case of evaluations at π in (5.8) we find that the resulting integral now becomes expressible in terms of gamma functions:

$$\begin{aligned} -\sum_{n,k\geqslant 0} \mathrm{Ls}_{n+k+1}^{(k)}(2\pi)\,\frac{\lambda^n}{n!}\frac{(i\mu)^k}{k!} &= \int_0^{2\pi}\left(2\sin\frac{\theta}{2}\right)^{\lambda}\mathrm{e}^{i\mu\theta}\,\mathrm{d}\theta \\ &= 2\pi\mathrm{e}^{i\mu\pi}\binom{\lambda}{\frac{\lambda}{2}+\mu} \end{aligned} \tag{5.13}$$

The special case $\mu = 0$, in the light of (5.18) which gives $\mathrm{Ls}_n(2\pi) = 2\,\mathrm{Ls}_n(\pi)$, recovers (5.4).

We may now extract log-sine integrals $\mathrm{Ls}_n^{(k)}(2\pi)$ in a similar way as described in Section 5.2.1.

Example 5.2.9. For instance,

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

We remark that this evaluation is incorrectly given in [Lew81, (7.144)] as $7\pi^5/30$ underscoring an advantage of automated evaluations over tables (indeed, there are more misprints in [Lew81] pointed out for instance in [DK01, KS05]). $\Diamond$

5.2.5 Log-sine-polylog integrals

Motivated by the integrals $\mathrm{LsLsc}_{k,i,j}$ defined in [Kal05] we show that the considerations of Section 5.2.3 can be extended to more involved integrals including

$$\mathrm{Ls}_n^{(k)}(\pi; d) := -\int_0^\pi \theta^k \log^{n-k-1}\left(2\sin\frac{\theta}{2}\right) \mathrm{Li}_d(\mathrm{e}^{i\theta})\,\mathrm{d}\theta.$$

On expressing $\mathrm{Li}_d(\mathrm{e}^{i\theta})$ as a series, rearranging, and applying Theorem 5.2.2, we obtain the following exponential generating function for $\mathrm{Ls}_n^{(k)}(\pi; d)$:

Corollary 5.2.10. *For $d \geqslant 0$ we have*

$$\begin{aligned} -\sum_{n,k\geqslant 0} \mathrm{Ls}_{n+k+1}^{(k)}(\pi; d)\,\frac{\lambda^n}{n!}\frac{(i\mu)^k}{k!} \\ = i\sum_{n\geqslant 1} H_{n,d}(\lambda)\frac{\mathrm{e}^{i\pi\frac{\lambda}{2}} - (-1)^n \mathrm{e}^{i\pi\mu}}{\mu - \frac{\lambda}{2} + n} \end{aligned} \tag{5.14}$$

where

$$H_{n,d}(\lambda) := \sum_{k=0}^{n-1} \frac{(-1)^k \binom{\lambda}{k}}{(n-k)^d}. \tag{5.15}$$

We note for $0 \leqslant \theta \leqslant \pi$ that $\mathrm{Li}_{-1}(\mathrm{e}^{i\theta}) = -1/\left(2\sin\frac{\theta}{2}\right)^2$, $\mathrm{Li}_0(\mathrm{e}^{i\theta}) = -\frac{1}{2} + \frac{i}{2}\cot\frac{\theta}{2}$, while $\mathrm{Li}_1(\mathrm{e}^{i\theta}) = -\log\left(2\sin\frac{\theta}{2}\right) + i\frac{\pi-\theta}{2}$, and $\mathrm{Li}_2(\mathrm{e}^{i\theta}) = \zeta(2) + \frac{\theta}{2}\left(\frac{\theta}{2} - \pi\right) + i\,\mathrm{Cl}_2(\theta)$.

Remark 5.2.11. Corresponding results for an arbitrary Dirichlet series $\mathrm{L}_{\mathbf{a},d}(x) := \sum_{n\geqslant 1} a_n x^n/n^d$ can be easily derived in the same fashion. Indeed, for

$$\mathrm{Ls}_n^{(k)}(\pi; \mathbf{a}, d) := -\int_0^\pi \theta^k \log^{n-k-1}\left(2\sin\frac{\theta}{2}\right) \mathrm{L}_{\mathbf{a},d}(\mathrm{e}^{i\theta})\,\mathrm{d}\theta$$

one derives the exponential generating function (5.14) with $H_{n,d}(\lambda)$ replaced by

$$H_{n,\mathbf{a},d}(\lambda) := \sum_{k=0}^{n-1} \frac{(-1)^k \binom{\lambda}{k} a_{n-k}}{(n-k)^d}. \tag{5.16}$$

This allows for $\mathrm{Ls}_n^{(k)}(\pi; \mathbf{a}, d)$ to be extracted for many number theoretic functions. It does not however seem to cover any of the values of the $\mathrm{LsLsc}_{k,i,j}$ function defined in [Kal05] that are not already covered by Corollary 5.2.10. $\diamondsuit$

5.3 Quasiperiodic properties

As shown in [Lew81, (7.1.24)], it follows from the periodicity of the integrand that, for integers m,

$$\begin{aligned}\mathrm{Ls}_n^{(k)}(2m\pi) &- \mathrm{Ls}_n^{(k)}(2m\pi - \sigma) \\ &= \sum_{j=0}^{k} (-1)^{k-j} (2m\pi)^j \binom{k}{j} \mathrm{Ls}_{n-j}^{(k-j)}(\sigma).\end{aligned} \tag{5.17}$$

Based on this quasiperiodic property of the log-sine integrals, the results of Section 5.2.4 easily generalize to show that log-sine integrals at multiples of 2π evaluate in terms of zeta values. This is shown in Section 5.3.1. It then follows from (5.17) that log-sine integrals at general arguments can be reduced to log-sine integrals at arguments $0 \leqslant \sigma \leqslant \pi$. This is discussed briefly in Section 5.3.2.

Example 5.3.1. In the case $k = 0$, we have that

$$\mathrm{Ls}_n(2m\pi) = 2m\,\mathrm{Ls}_n(\pi). \tag{5.18}$$

For $k=1$, specializing (5.17) to $\sigma = 2m\pi$ then yields

$$\operatorname{Ls}_n^{(1)}(2m\pi) = 2m^2\pi \operatorname{Ls}_{n-1}(\pi)$$

as is given in [Lew81, (7.1.23)]. $\diamondsuit$

5.3.1 Log-sine integrals at multiples of 2π

For odd k, specializing (5.17) to $\sigma = 2m\pi$, we find

$$2\operatorname{Ls}_n^{(k)}(2m\pi) = \sum_{j=1}^{k} (-1)^{j-1} (2m\pi)^j \binom{k}{j} \operatorname{Ls}_{n-j}^{(k-j)}(2m\pi)$$

giving $\operatorname{Ls}_n^{(k)}(2m\pi)$ in terms of lower order log-sine integrals.

More generally, on setting $\sigma = 2\pi$ in (5.17) and summing the resulting equations for increasing m in a telescoping fashion, we arrive at the following reduction. We will use the standard notation

$$H_n^{(a)} := \sum_{k=1}^{n} k^{-a}$$

for *generalized harmonic sums.*

Theorem 5.3.2. *For integers $m \geqslant 0$,*

$$\operatorname{Ls}_n^{(k)}(2m\pi) = \sum_{j=0}^{k} (-1)^{k-j} (2\pi)^j \binom{k}{j} H_m^{(-j)} \operatorname{Ls}_{n-j}^{(k-j)}(2\pi).$$

Summarizing, we have thus shown that the generalized log-sine integrals at multiples of 2π may always be evaluated in terms of integrals at 2π. In particular, $\operatorname{Ls}_n^{(k)}(2m\pi)$ can always be evaluated in terms of zeta values by the methods of Section 5.2.4.

5.3.2 Reduction of arguments

A general (real) argument σ can be written uniquely as $\sigma = 2m\pi \pm \sigma_0$ where $m \geqslant 0$ is an integer and $0 \leqslant \sigma_0 \leqslant \pi$. It then follows from (5.17) and

$$\mathrm{Ls}_n^{(k)}(-\theta) = (-1)^{k+1}\,\mathrm{Ls}_n^{(k)}(\theta)$$

that $\mathrm{Ls}_n^{(k)}(\sigma)$ equals

$$\mathrm{Ls}_n^{(k)}(2m\pi) \pm \sum_{j=0}^{k}(\pm 1)^{k-j}(2m\pi)^j\binom{k}{j}\mathrm{Ls}_{n-j}^{(k-j)}(\sigma_0)\,. \tag{5.19}$$

Since the evaluation of log-sine integrals at multiples of 2π was explicitly treated in Section 5.3.1 this implies that the evaluation of log-sine integrals at general arguments σ reduces to the case of arguments $0 \leqslant \sigma \leqslant \pi$.

5.4 Evaluations at other values

In this section we first discuss a method for evaluating the generalized log-sine integrals at arbitrary arguments in terms of Nielsen polylogarithms at related arguments. The gist of our technique originates with Fuchs ([Fuc61], [Lew81, §7.10]). Related evaluations appear in [DK00] for $\mathrm{Ls}_3(\tau)$ to $\mathrm{Ls}_6(\tau)$ as well as in [DK01] for $\mathrm{Ls}_n(\tau)$ and $\mathrm{Ls}_n^{(1)}(\tau)$.

We then specialize to evaluations at $\pi/3$ in Section 5.4.1. The polylogarithms arising in this case have been studied under the name of *multiple Clausen and Glaisher values* in [BBK01]. In fact, the next result (5.20) with $\tau = \pi/3$ is a modified version of [BBK01, Lemma 3.2]. We employ the notation

$$\binom{n}{a_1, \ldots, a_k} := \frac{n!}{a_1! \cdots a_k!(n - a_1 - \ldots - a_k)!}$$

for multinomial coefficients.

Theorem 5.4.1. *For $0 \leqslant \tau \leqslant 2\pi$, and nonnegative integers n, k such that $n-k \geqslant 2$,*

$$\begin{aligned} \zeta(n-k,\{1\}^k) &- \sum_{j=0}^{k} \frac{(-i\tau)^j}{j!} \operatorname{Li}_{2+k-j,\{1\}^{n-k-2}}(\mathrm{e}^{i\tau}) \\ &= \frac{i^{k+1}(-1)^{n-1}}{(n-1)!} \sum_{r=0}^{n-k-1} \sum_{m=0}^{r} \binom{n-1}{k,m,r-m} \\ &\quad \times \left(\frac{i}{2}\right)^r (-\pi)^{r-m} \operatorname{Ls}_{n-(r-m)}^{(k+m)}(\tau)\,. \end{aligned} \tag{5.20}$$

Proof. Starting with

$$\operatorname{Li}_{k,\{1\}^n}(\alpha) - \operatorname{Li}_{k,\{1\}^n}(1) = \int_1^\alpha \frac{\operatorname{Li}_{k-1,\{1\}^n}(z)}{z}\,\mathrm{d}z$$

and integrating by parts repeatedly, we obtain

$$\begin{aligned} \sum_{j=0}^{k-2} \frac{(-1)^j}{j!} \log^j(\alpha) \operatorname{Li}_{k-j,\{1\}^n}(\alpha) &- \operatorname{Li}_{k,\{1\}^n}(1) \\ &= \frac{(-1)^{k-2}}{(k-2)!} \int_1^\alpha \frac{\log^{k-2}(z) \operatorname{Li}_{\{1\}^{n+1}}(z)}{z}\,\mathrm{d}z. \end{aligned} \tag{5.21}$$

Letting $\alpha = \mathrm{e}^{i\tau}$ and changing variables to $z = \mathrm{e}^{i\theta}$, as well as using

$$\operatorname{Li}_{\{1\}^n}(z) = \frac{(-\log(1-z))^n}{n!},$$

the right-hand side of (5.21) can be rewritten as

$$\frac{(-1)^{k-2}}{(k-2)!} \frac{i}{(n+1)!} \int_0^\tau (i\theta)^{k-2} \left(-\log\left(1-\mathrm{e}^{i\theta}\right)\right)^{n+1} \mathrm{d}\theta.$$

Since, for $0 \leqslant \theta \leqslant 2\pi$ and the principal branch of the logarithm,

$$\log(1-\mathrm{e}^{i\theta}) = \log\left|2\sin\frac{\theta}{2}\right| + \frac{i}{2}(\theta-\pi), \tag{5.22}$$

this last integral can now be expanded in terms of generalized log-sine integrals at τ.

$$\begin{aligned}\zeta(k,\{1\}^n) &- \sum_{j=0}^{k-2}\frac{(-i\tau)^j}{j!}\operatorname{Li}_{k-j,\{1\}^n}(\mathrm{e}^{i\tau})\\ &= \frac{(-i)^{k-1}}{(k-2)!}\frac{(-1)^n}{(n+1)!}\sum_{r=0}^{n+1}\sum_{m=0}^{r}\binom{n+1}{r}\binom{r}{m}\\ &\qquad \left(\frac{i}{2}\right)^r(-\pi)^{r-m}\operatorname{Ls}_{n+k-(r-m)}^{(k+m-2)}(\tau)\,. \end{aligned} \tag{5.23}$$

Applying the *MZV duality formula* [BBBL01], we have

$$\zeta(k,\{1\}^n) = \zeta(n+2,\{1\}^{k-2}),$$

and a change of variables yields the claim. □

We recall that the real and imaginary parts of the multiple polylogarithms are Clausen and Glaisher functions as defined in (1.14) and (1.15).

Example 5.4.2. Applying (5.20) with $n = 4$ and $k = 1$ and solving for $\operatorname{Ls}_4^{(1)}(\tau)$ yields

$$\begin{aligned}\operatorname{Ls}_4^{(1)}(\tau) &= 2\zeta(3,1) - 2\operatorname{Gl}_{3,1}(\tau) - 2\tau\operatorname{Gl}_{2,1}(\tau)\\ &\quad + \frac{1}{4}\operatorname{Ls}_4^{(3)}(\tau) - \frac{1}{2}\pi\operatorname{Ls}_3^{(2)}(\tau) + \frac{1}{4}\pi^2\operatorname{Ls}_2^{(1)}(\tau)\\ &= \frac{1}{180}\pi^4 - 2\operatorname{Gl}_{3,1}(\tau) - 2\tau\operatorname{Gl}_{2,1}(\tau)\\ &\quad - \frac{1}{16}\tau^4 + \frac{1}{6}\pi\tau^3 - \frac{1}{8}\pi^2\tau^2.\end{aligned}$$

For the last equality we used the trivial evaluation

$$\operatorname{Ls}_n^{(n-1)}(\tau) = -\frac{\tau^n}{n}. \tag{5.24}$$

It appears that both $\mathrm{Gl}_{2,1}(\tau)$ and $\mathrm{Gl}_{3,1}(\tau)$ are not reducible for $\tau = \pi/2$ or $\tau = 2\pi/3$. Here, reducible means expressible in terms of multi zeta values and Glaisher functions of the same argument and lower weight. In the case $\tau = \pi/3$ such reductions are possible. This is discussed in Example 5.4.5 and illustrates how much less simple values at $2\pi/3$ are than those at $\pi/3$. We remark, however, that $\mathrm{Gl}_{2,1}(2\pi/3)$ is reducible to one-dimensional polylogarithmic terms [BS11a]. In [BBSW12] explicit reductions for all weight four or less polylogarithms are given. $\diamondsuit$

Remark 5.4.3. Lewin [Lew81, 7.4.3] uses the special case $k = n-2$ of (5.20) to deduce a few small integer evaluations of the log-sine integrals $\mathrm{Ls}_n^{(n-2)}(\pi/3)$ in terms of classical Clausen functions. $\diamondsuit$

In general, we can use (5.20) recursively to express the log-sine values $\mathrm{Ls}_n^{(k)}(\tau)$ in terms of multiple Clausen and Glaisher functions at τ.

Example 5.4.4. (5.20) with $n = 5$ and $k = 1$ produces

$$\begin{aligned}\mathrm{Ls}_5^{(1)}(\tau) &= -6\zeta(4,1) + 6\,\mathrm{Cl}_{3,1,1}(\tau) + 6\tau\,\mathrm{Cl}_{2,1,1}(\tau)\\ &\quad + \frac{3}{4}\mathrm{Ls}_5^{(3)}(\tau) - \frac{3}{2}\pi\,\mathrm{Ls}_4^{(2)}(\tau) + \frac{3}{4}\pi^2\,\mathrm{Ls}_3^{(1)}(\tau).\end{aligned}$$

Applying (5.20) three more times to rewrite the remaining log-sine integrals produces an evaluation of $\mathrm{Ls}_5^{(1)}(\tau)$ in terms of multi zeta values and Clausen functions at τ. $\diamondsuit$

5.4.1 Log-sine integrals at $\pi/3$

We now apply the general results obtained in Section 5.4 to the evaluation of log-sine integrals at $\tau = \pi/3$. Accordingly, we encounter multiple polylogarithms at the basic 6-th root of unity $\omega := \exp(i\pi/3)$. Their real and imaginary parts satisfy various relations and reductions, studied in [BBK01], which allow us to further treat the resulting evaluations. In general, these polylogarithms are more tractable than those at other values because $\overline{\omega} = \omega^2$.

Example 5.4.5. (Values at $\frac{\pi}{3}$) Continuing Example 5.4.2 we have

$$-\operatorname{Ls}_4^{(1)}\left(\frac{\pi}{3}\right) = 2\operatorname{Gl}_{3,1}\left(\frac{\pi}{3}\right) + \frac{2}{3}\pi\operatorname{Gl}_{2,1}\left(\frac{\pi}{3}\right) + \frac{19}{6480}\pi^4.$$

Using known reductions from [BBK01] we get:

$$\operatorname{Gl}_{2,1}\left(\frac{\pi}{3}\right) = \frac{1}{324}\pi^3, \quad \operatorname{Gl}_{3,1}\left(\frac{\pi}{3}\right) = -\frac{23}{19440}\pi^4, \tag{5.25}$$

and so arrive at

$$-\operatorname{Ls}_4^{(1)}\left(\frac{\pi}{3}\right) = \frac{17}{6480}\pi^4. \tag{5.26}$$

Lewin explicitly mentions (5.26) in the preface to [Lew81] because of its "queer" nature which he compares to some of Landen's curious 18th century formulas. $\diamondsuit$

Many more reduction besides (5.25) are known. In particular, the one-dimensional Glaisher and Clausen functions reduce as follows [Lew81]:

$$\begin{aligned}
\operatorname{Gl}_n(2\pi x) &= \frac{2^{n-1}(-1)^{1+\lfloor n/2\rfloor}}{n!}B_n(x)\,\pi^n, \\
\operatorname{Cl}_{2n+1}\left(\frac{\pi}{3}\right) &= \frac{1}{2}(1-2^{-2n})(1-3^{-2n})\zeta(2n+1).
\end{aligned} \tag{5.27}$$

Here, B_n denotes the n-th *Bernoulli polynomial*. Further reductions can be derived for instance from the duality result [BBK01, Theorem 4.4]. For low dimensions, we have built these reductions into our program, see Section 5.5.

Example 5.4.6. (Values of $\mathrm{Ls}_n\,(\pi/3)$) The log-sine integrals at $\pi/3$ are evaluated by our program as follows:

$$\begin{aligned}
\mathrm{Ls}_2\left(\frac{\pi}{3}\right) &= \mathrm{Cl}_2\left(\frac{\pi}{3}\right)\\
-\mathrm{Ls}_3\left(\frac{\pi}{3}\right) &= \frac{7}{108}\,\pi^3\\
\mathrm{Ls}_4\left(\frac{\pi}{3}\right) &= \frac{1}{2}\pi\,\zeta(3) + \frac{9}{2}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right)\\
-\mathrm{Ls}_5\left(\frac{\pi}{3}\right) &= \frac{1543}{19440}\pi^5 - 6\,\mathrm{Gl}_{4,1}\left(\frac{\pi}{3}\right)\\
\mathrm{Ls}_6\left(\frac{\pi}{3}\right) &= \frac{15}{2}\pi\,\zeta(5) + \frac{35}{36}\,\pi^3\zeta(3) + \frac{135}{2}\,\mathrm{Cl}_6\left(\frac{\pi}{3}\right)\\
-\mathrm{Ls}_7\left(\frac{\pi}{3}\right) &= \frac{74369}{326592}\pi^7 + \frac{15}{2}\,\pi\zeta(3)^2 - 135\;\mathrm{Gl}_{6,1}\left(\frac{\pi}{3}\right)
\end{aligned}$$

As follows from the results of Section 5.4 each integral is a multivariable rational polynomial in π as well as Cl, Gl, and zeta values. These evaluations confirm those given in [DK01, Appendix A] for $\mathrm{Ls}_3\left(\frac{\pi}{3}\right)$, $\mathrm{Ls}_4\left(\frac{\pi}{3}\right)$, and $\mathrm{Ls}_6\left(\frac{\pi}{3}\right)$. Less explicitely, the evaluations of $\mathrm{Ls}_5\left(\frac{\pi}{3}\right)$ and $\mathrm{Ls}_7\left(\frac{\pi}{3}\right)$ can be recovered from similar results in [KS05, DK01] (which in part were obtained using PSLQ; we refer to Section 5.5 for how our analysis relies on PSLQ).

The first presumed-irreducible value that occurs is

$$\begin{aligned}
\mathrm{Gl}_{4,1}\left(\frac{\pi}{3}\right) &= \sum_{n=1}^{\infty} \frac{\sum_{k=1}^{n-1}\frac{1}{k}}{n^4}\,\sin\left(\frac{n\pi}{3}\right)\\
&= \frac{3341}{1632960}\pi^5 - \frac{1}{\pi}\zeta(3)^2 - \frac{3}{4\pi}\sum_{n=1}^{\infty}\frac{1}{\binom{2n}{n}n^6}.
\end{aligned} \tag{5.28}$$

The final evaluation is described in [BBK01]. Extensive computation suggests it is not expressible as a sum of products of one dimensional Glaisher and zeta values. Indeed, conjectures are made in [BBK01, §5] for the number of irreducibles at each depth. Related dimensional conjectures for polylogs are discussed in [Zlo07]. ◊

5.4.2 Log-sine integrals at imaginary values

The approach of Section 5.4 may be extended to evaluate log-sine integrals at imaginary arguments. In more usual terminology, these are *log-sinh integrals*

$$\mathrm{Lsh}_n^{(k)}(\sigma) := -\int_0^\sigma \theta^k \log^{n-1-k}\left|2\sinh\frac{\theta}{2}\right| \mathrm{d}\theta \tag{5.29}$$

which are related to log-sine integrals by

$$\mathrm{Lsh}_n^{(k)}(\sigma) = (-i)^{k+1}\,\mathrm{Ls}_n^{(k)}(i\sigma).$$

We may derive a result along the lines of Theorem 5.4.1 by observing that equation (5.22) is replaced, when $\theta = it$ for $t > 0$, by the simpler

$$\log(1-\mathrm{e}^{-t}) = \log\left|2\sinh\frac{t}{2}\right| - \frac{t}{2}. \tag{5.30}$$

This leads to:

Theorem 5.4.7. *For $t > 0$, and nonnegative integers n, k such that $n-k \geqslant 2$,*

$$\begin{aligned}\zeta(n-k,\{1\}^k) &- \sum_{j=0}^{k} \frac{t^j}{j!}\,\mathrm{Li}_{2+k-j,\{1\}^{n-k-2}}(\mathrm{e}^{-t}) \\ &= \frac{(-1)^{n+k}}{(n-1)!} \sum_{r=0}^{n-k-1} \binom{n-1}{k,r} \left(-\frac{1}{2}\right)^r \mathrm{Lsh}_n^{(k+r)}(t).\end{aligned} \tag{5.31}$$

Example 5.4.8. Let $\rho := (1+\sqrt{5})/2$ be the golden mean. Then, by applying Theorem 5.4.7 with $n = 3$ and $k = 1$,

$$\begin{aligned}\mathrm{Lsh}_3^{(1)}(2\log\rho) = \zeta(3) &- \frac{4}{3}\log^3\rho \\ &- \mathrm{Li}_3(\rho^{-2}) - 2\,\mathrm{Li}_2(\rho^{-2})\log\rho.\end{aligned}$$

This may be further reduced, using $\mathrm{Li}_2(\rho^{-2}) = \frac{\pi^2}{15} - \log^2\rho$ and $\mathrm{Li}_3(\rho^{-2}) = \frac{4}{5}\zeta(3) - \frac{2}{15}\pi^2\log\rho + \frac{2}{3}\log^3\rho$, to yield the well-known

$$\mathrm{Lsh}_3^{(1)}(2\log\rho) = \frac{1}{5}\zeta(3).$$

The interest in this kind of evaluation stems from the fact that log-sinh integrals at $2\log\rho$ express values of alternating inverse binomial sums (the fact that log-sine integrals at $\pi/3$ give inverse binomial sums is illustrated by Example 5.4.6 and (5.28)). In this case,

$$\mathrm{Lsh}_3^{(1)}(2\log\rho) = \frac{1}{2}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{\binom{2n}{n}n^3}.$$

More on this relation and generalizations can be found in each of [NYW95, KV00, BBK01, BBG04]. ♢

5.5 Reducing polylogarithms

The techniques described in Sections 5.2.3 and 5.4 for evaluating log-sine integrals in terms of multiple polylogarithms usually produce expressions that can be considerably reduced as is illustrated in Examples 5.2.6, 5.2.7, and 5.4.5. Relations between polylogarithms have been the subject of many studies [BBBL01, BBG04] with a special focus on (alternating) multiple zeta values [Köl82, HO03, Zlo07] and, to a lesser extent, Clausen values [BBK01].

There is a certain deal of choice in how to combine the various techniques that we present in order to evaluate log-sine integrals at certain values. The next example shows how this can be exploited to derive relations among the various polylogarithms involved.

Example 5.5.1. For $n = 5$ and $k = 2$, specializing (5.17) to $\sigma = \pi$ and $m = 1$ yields

$$\mathrm{Ls}_5^{(2)}(2\pi) = 2\,\mathrm{Ls}_5^{(2)}(\pi) - 4\pi\,\mathrm{Ls}_4^{(1)}(\pi) + 4\pi^2\,\mathrm{Ls}_3(\pi).$$

By Example 5.2.9 we know that this evaluates as $-13/45\pi^5$. On the other hand, we may use the technique of Section 5.2.3 to reduce the log-sine integrals at π. This leads to

$$-8\pi\,\mathrm{Li}_{3,1}(1) + 12\pi\,\mathrm{Li}_4(1) - \frac{2}{5}\pi^5 = -\frac{13}{45}\pi^5.$$

In simplified terms, we have derived the famous identity $\zeta(3,1) = \frac{\pi^4}{360}$. Similarly, the case $n = 6$ and $k = 2$ leads to $\zeta(3,1,1) = \frac{3}{2}\zeta(4,1) + \frac{1}{12}\pi^2\zeta(3) - \zeta(5)$ which further reduces to $2\zeta(5) - \frac{\pi^2}{6}\zeta(3)$. As a final example, the case $n = 7$ and $k = 4$ produces $\zeta(5,1) = \frac{\pi^6}{1260} - \frac{1}{2}\zeta(3)^2$. ◊

For the purpose of an implementation, we have built many reductions of multiple polylogarithms into our program. Besides some general rules, such as (5.27), the program contains a table of reductions at low weight for polylogarithms at the values 1 and -1, as well as Clausen and Glaisher functions at the values $\pi/2$, $\pi/2$, and $2\pi/3$. These correspond to the polylogarithms that occur in the evaluation of the log-sine integrals at the special values $\pi/3$, $\pi/2$, $2\pi/3$, π which are of particular importance for applications as mentioned in the introduction. This table of reductions has been compiled using the integer relation finding algorithm PSLQ [BBG04]. Its use is thus of heuristic nature (as opposed to the rest of the program which is working symbolically from the analytic results in this paper) and is therefore made optional.

5.6 The program

5.6.1 Basic usage

As promised, we implemented[1] the presented results for evaluating log-sine integrals for use in the computer algebra systems *Mathematica* and SAGE. The basic usage is very simple and illustrated in the next example for *Mathematica*[2].

Example 5.6.1. Consider the log-sine integral $\mathrm{Ls}_5^{(2)}(2\pi)$. The following self-explanatory code evaluates it in terms of polylogarithms:

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

This produces the output $-13/45\pi^5$ as in Example 5.2.9. As a second example,

```
-LsToLi[Ls[5,0,Pi/3]]
```

results in the output

```
1543/19440*Pi^5 - 6*Gl[{4,1},Pi/3]
```

which agrees with the evaluation in Example 5.4.6. Finally,

```
LsToLi[Ls[5,1,Pi]]
```

produces

```
6*Li[{3,1,1},-1] + (Pi^2*Zeta[3])/4
- (105*Zeta[5])/32
```

as in Example 5.2.6. $\diamondsuit$

---

[1]The packages are freely available for download from
http://arminstraub.com/pub/log-sine-integrals

[2]The interface in the case of SAGE is similar but may change slightly, especially as we hope to integrate our package into the core of SAGE.

Example 5.6.2. Computing

```
LsToLi[Ls[6,3,Pi/3]-2*Ls[6,1,Pi/3]]
```

yields the value $\frac{313}{204120}\pi^6$ and thus automatically proves a result of Zucker [Zuc85]. A family of relations between log-sine integrals at $\pi/3$ generalizing the above has been established in [NYW95]. $\Diamond$

5.6.2 Implementation

The conversion from log-sine integrals to polylogarithmic values demonstrated in Example 5.6.1 roughly proceeds as follows:

- First, the evaluation of $\mathrm{Ls}_n^{(k)}(\sigma)$ is reduced to the cases of $0 \leqslant \sigma \leqslant \pi$ and $\sigma = 2m\pi$ as described in Section 5.3.2.
- The cases $\sigma = 2m\pi$ are treated as in Section 5.2.4 and result in multiple zeta values.
- The other cases σ result in polylogarithmic values at $e^{i\sigma}$ and are obtained using the results of Sections 5.2.3 and 5.4.
- Finally, especially in the physically relevant cases, various reductions of the resulting polylogarithms are performed as outlined in Section 5.5.

5.6.3 Numerical usage

The program is also useful for numerical computations provided that it is coupled with efficient methods for evaluating polylogarithms to high precision. It complements for instance the C++ library `lsjk` “for arbitrary-precision numeric evaluation of the generalized log-sine functions” described in [KS05].

Example 5.6.3. We evaluate

$$\operatorname{Ls}_5^{(2)}\left(\frac{2\pi}{3}\right) = 4\,\operatorname{Gl}_{4,1}\left(\frac{2\pi}{3}\right) - \frac{8}{3}\pi\,\operatorname{Gl}_{3,1}\left(\frac{2\pi}{3}\right) - \frac{8}{9}\pi^2\,\operatorname{Gl}_{2,1}\left(\frac{2\pi}{3}\right) - \frac{8}{1215}\pi^5.$$

Using specialized code[3] such as [VW05], the right-hand side is readily evaluated to, for instance, two thousand digit precision in about a minute. The first 1024 digits of the result match the evaluation given in [KS05]. However, due to its implementation `lsjk` currently is restricted to log-sine functions $\operatorname{Ls}_n^{(k)}(\theta)$ with $k \leqslant 9$. ♢

[3]The C++ code we used is based on the fast Hölder transform described in [BBBL01], and is available on request.

Chapter 6

Log-sine evaluations of Mahler measures

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[BS11a] *Log-sine evaluations of Mahler measures*
(with Jonathan M. Borwein)
to appear in Journal of the Australian Mathematical Society

Abstract We provide evaluations of several recently studied higher and multiple Mahler measures using log-sine integrals. This is complemented with an analysis of generating functions and identities for log-sine integrals which allows the evaluations to be expressed in terms of zeta values or more general polylogarithmic terms. The machinery developed is then applied to evaluation of further families of multiple Mahler measures.

6.1 Preliminaries

For k functions (typically Laurent polynomials) in n variables the *multiple Mahler measure*, introduced in [KLO08], is defined by

$$\mu(P_1, P_2, \ldots, P_k) := \int_0^1 \cdots \int_0^1 \prod_{j=1}^{k} \log \left| P_j \left(e^{2\pi i t_1}, \ldots, e^{2\pi i t_n} \right) \right| \mathrm{d}t_1 \mathrm{d}t_2 \ldots \mathrm{d}t_n.$$

When $P = P_1 = P_2 = \cdots = P_k$ this devolves to the *higher Mahler measure*, $\mu_k(P)$, as introduced and examined in [KLO08]. When $k = 1$ both reduce to the standard (logarithmic) *Mahler measure* [Boy81].

For $n = 1, 2, \ldots$, we consider the *log-sine integrals* defined by

$$\mathrm{Ls}_n\left(\sigma\right) := -\int_0^{\sigma} \log^{n-1}\left|2\,\sin\frac{\theta}{2}\right|\,\mathrm{d}\theta \tag{6.1}$$

and their moments for $k \geqslant 0$ given by

$$\mathrm{Ls}_n^{(k)}\left(\sigma\right) := -\int_0^{\sigma} \theta^k\,\log^{n-1-k}\left|2\,\sin\frac{\theta}{2}\right|\,\mathrm{d}\theta. \tag{6.2}$$

This is the notation used by Lewin [Lew58, Lew81], and the integrals in (6.2) are usually referred to as *generalized log-sine integrals*. Note that in each case the modulus is not needed for $0 \leqslant \sigma \leqslant 2\pi$. Various log-sine integral evaluations may be found in Lewin's book [Lew81, §7.6 & §7.9].

We observe that $\mathrm{Ls}_1\left(\sigma\right) = -\sigma$ and that $\mathrm{Ls}_n^{(0)}\left(\sigma\right) = \mathrm{Ls}_n\left(\sigma\right)$. In particular,

$$\mathrm{Ls}_2\left(\sigma\right) = \mathrm{Cl}_2\left(\sigma\right) := \sum_{n=1}^{\infty} \frac{\sin(n\sigma)}{n^2} \tag{6.3}$$

is the *Clausen function* which plays a prominent role below. Generalized Clausen functions are introduced in (1.14).

Remark 6.1.1. We remark that it is fitting given the dedication of this article and volume that Alf van der Poorten wrote the foreword to Lewin's "bible" [Lew81]. In fact, he enthusiastically mentions the evaluation

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

and its relation with inverse central binomial sums. This will be explained in Example 6.2.5. Evaluations of log-sine integrals at $\pi/3$ are discussed in Section 6.2.2. $\Diamond$

Example 6.1.2 (Two classical Mahler measures revisited)**.** As we will have recourse to the methods used in this example, we reevaluate $\mu(1+x+y)$ and $\mu(1+x+y+z)$. The starting point is *Jensen's formula*:

$$\int_0^1 \log\left|\alpha + e^{2\pi i\, t}\right|\, \mathrm{d}t = \log\left(\max\{|\alpha|, 1\}\right). \tag{6.4}$$

To evaluate $\mu(1+x+y)$, we use (6.4) to obtain

$$\mu(1+x+y) = \int_{1/6}^{5/6} \log(2\sin(\pi y))\, \mathrm{d}y = \frac{1}{\pi}\,\mathrm{Ls}_2\left(\frac{\pi}{3}\right) = \frac{1}{\pi}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right), \tag{6.5}$$

which is a form of Smyth's seminal 1981 result, see [Boy81, Appendix 1].

To evaluate $\mu(1+x+y+z)$, we follow Boyd [Boy81, Appendix 1] and observe, on applying Jensen's formula, that for complex constants a and b

$$\mu(ax+b) = \log|a| \vee \log|b|. \tag{6.6}$$

Writing $w = y/z$ we have

$$\begin{aligned}
\mu(1+x+y+z) &= \mu(1+x+z(1+w)) = \mu(\log|1+w| \vee \log|1+x|) \\
&= \frac{1}{\pi^2}\int_0^\pi \mathrm{d}\theta \int_0^\pi \max\left\{\log\left(2\sin\frac{\theta}{2}\right), \log\left(2\sin\frac{t}{2}\right)\right\}\, \mathrm{d}t \\
&= \frac{2}{\pi^2}\int_0^\pi \mathrm{d}\theta \int_0^\theta \log\left(2\sin\frac{\theta}{2}\right)\, \mathrm{d}t \\
&= \frac{2}{\pi^2}\int_0^\pi \theta\log\left(2\sin\frac{\theta}{2}\right)\, \mathrm{d}\theta \\
&= -\frac{2}{\pi^2}\,\mathrm{Ls}_3^{(1)}(\pi) = \frac{7}{2}\frac{\zeta(3)}{\pi^2}.
\end{aligned} \tag{6.7}$$

The final result is again due originally to Smyth. $\Diamond$

6.2 Log-sine integrals at π and $\pi/3$

The multiple Mahler measure

$$\mu_k(1+x+y_*) := \mu(1+x+y_1, 1+x+y_2, \ldots, 1+x+y_k) \tag{6.8}$$

was studied by Sasaki [Sas10, (4.1)]. He uses Jensen's formula (6.4) to observe that

$$\mu_k(1+x+y_*) = \int_{1/6}^{5/6} \log^k \left|1 - e^{2\pi i\, t}\right| \,\mathrm{d}t \tag{6.9}$$

and so provides an evaluation of $\mu_2(1+x+y_*)$. On the other hand, immediately from (6.9) and the definition (6.1) of the log-sine integrals we have:

Theorem 6.2.1. *For positive integers k,*

$$\mu_k(1+x+y_*) = \frac{1}{\pi}\,\mathrm{Ls}_{k+1}\left(\frac{\pi}{3}\right) - \frac{1}{\pi}\,\mathrm{Ls}_{k+1}\left(\pi\right). \tag{6.10}$$

In Sections 6.2.1 and 6.2.2 we will cultivate Theorem 6.2.1 by showing how to recursively evaluate the log-sine integrals at π and $\pi/3$ respectively. In view of Theorem 6.2.1 this then provides evaluations of all multiple Mahler measures $\mu_k(1+x+y_*)$ as is made explicit in Section 6.3.1.

Further Mahler measure evaluations given later in this paper will further involve the generalized log-sine integrals, defined in (6.2), at π. These are studied in Section 6.2.3.

6.2.1 Log-sine integrals at π

First, [Lew58, Eqn (8)] provides

$$\mathrm{Ls}_{n+2}(\pi) = (-1)^n n! \left(\pi\, \alpha(n+1) + \sum_{k=1}^{n-2} \frac{(-1)^k}{(k+1)!}\, \alpha(n-k)\, \mathrm{Ls}_{k+2}(\pi) \right), \tag{6.11}$$

where $\alpha(m) = (1-2^{1-m})\zeta(m)$. Note that $\alpha(1) = 0$ while for $m \geqslant 2$

$$\alpha(m) = -\operatorname{Li}_m(-1) = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^m}.$$

This is a consequence of the exponential generating function [Lew81, Eqn. (7.109)] for the requisite log-sine integrals:

$$-\sum_{m=0}^{\infty} \mathrm{Ls}_{m+1}(\pi)\, \frac{x^m}{m!} = \pi \frac{\Gamma(1+x)}{\Gamma^2\left(1+\frac{x}{2}\right)} = \pi \binom{x}{x/2}. \tag{6.12}$$

This will be revisited and explained in Section 6.4.1.

Example 6.2.2 (Values of $\mathrm{Ls}_n(\pi)$)**.** We have $\mathrm{Ls}_2(\pi) = 0$ and

$$\begin{aligned}
-\mathrm{Ls}_3(\pi) &= \frac{1}{12}\pi^3, \\
\mathrm{Ls}_4(\pi) &= \frac{3}{2}\pi\,\zeta(3), \\
-\mathrm{Ls}_5(\pi) &= \frac{19}{240}\pi^5, \\
\mathrm{Ls}_6(\pi) &= \frac{45}{2}\pi\,\zeta(5) + \frac{5}{4}\pi^3\zeta(3), \\
-\mathrm{Ls}_7(\pi) &= \frac{275}{1344}\pi^7 + \frac{45}{2}\pi\,\zeta^2(3), \\
\mathrm{Ls}_8(\pi) &= \frac{2835}{4}\pi\,\zeta(7) + \frac{315}{8}\pi^3\zeta(5) + \frac{133}{32}\pi^5\zeta(3),
\end{aligned}$$

and so forth. The fact that each integral is a multi-variable rational polynomial in π and zeta values follows directly from the recursion (6.11). Alternatively, these values may be conveniently obtained from (6.12) by a computer algebra system as the following snippet of *Maple* code demonstrates:

```
for k to 7 do simplify(subs(x=0,diff(Pi*binomial(x,x/2),x$k))) od
```
◊

6.2.2 Log-sine integrals at $\pi/3$

In this section, we turn to the log-sine integrals integrals at $\pi/3$. It is shown in [BS11c] that the log-sine integrals $\mathrm{Ls}_n^{(k)}(\tau)$ can be evaluated in terms of zeta values with the addition of multiple Clausen and Glaisher functions at τ. The gist of the technique originates with Fuchs ([Fuc61], [Lew81, §7.10]). In the case $\tau = \pi/3$ the resulting evaluations usually allow considerable reductions. This is because the basic sixth root of unity $\omega = \mathrm{e}^{i\pi/3}$ satisfies $\overline{\omega} = \omega^2$. As a consequence, the log-sine integrals $\mathrm{Ls}_n^{(k)}(\pi/3)$ are more tractable than those at other values; which fact we illustrate next.

Example 6.2.3 (Reducibility)**.** Proceeding as in [BS11c], in addition to $\mathrm{Ls}_n^{(n-1)}(\tau) = -\tau^n/n$ and $\mathrm{Ls}_2(\tau) = \mathrm{Cl}_2(\tau)$, we have

$$\begin{aligned} -\mathrm{Ls}_3(\tau) &= 2\,\mathrm{Gl}_{2,1}(\tau) + \frac{1}{12}\tau(3\pi^2 - 3\pi\tau + \tau^2) \\ \mathrm{Ls}_3^{(1)}(\tau) &= \mathrm{Cl}_3(\tau) + \tau\,\mathrm{Cl}_2(\tau) - \zeta(3), \end{aligned}$$

as well as

$$\begin{aligned} -\mathrm{Ls}_4(\tau) &= -6\,\mathrm{Cl}_{2,1,1}(\tau) + \frac{3}{2}\mathrm{Cl}_4(\tau) + \frac{3}{2}(\pi-\tau)\,\mathrm{Cl}_3(\tau) - \frac{3}{4}(\pi-\tau)^2\,\mathrm{Cl}_2(\tau) - \frac{3}{2}\pi\zeta(3), \\ \mathrm{Ls}_4^{(1)}(\tau) &= \frac{1}{180}\pi^4 - \frac{1}{16}\tau^4 + \frac{1}{6}\pi\tau^3 - \frac{1}{8}\pi^2\tau^2 - 2\,\mathrm{Gl}_{3,1}(\tau) - 2\tau\,\mathrm{Gl}_{2,1}(\tau), \\ \mathrm{Ls}_4^{(2)}(\tau) &= -2\,\mathrm{Cl}_4(\tau) + 2\tau\,\mathrm{Cl}_3(\tau) + \tau^2\,\mathrm{Cl}_2(\tau). \end{aligned}$$

In the case $\tau = \pi/3$ these evaluations can be further reduced as will be shown in Example 6.2.4. On the other hand, it appears that, for instance, $\mathrm{Gl}_{2,1}(\tau)$ is not reducible even for the special values $\tau = \pi/2$ or $\tau = 2\pi/3$. Here, reducible means expressible in terms of multi zeta values and Glaisher (resp. Clausen) functions of the same argument and lower weight. Yet, $\mathrm{Gl}_{2,1}(2\pi/3)$ is reducible to one-dimensional polylogarithmic terms at different arguments as will be shown in (6.59).

More generally, in [BBSW12] explicit reductions for all weight-four-or-less polylogarithms are given. ♢

Example 6.2.4 (Values of $\mathrm{Ls}_n(\pi/3)$)**.** The following evaluations may be obtained with the help of the implementation[1] accompanying [BS11c]:

$$\begin{aligned}
\mathrm{Ls}_2\left(\frac{\pi}{3}\right) &= \mathrm{Cl}_2\left(\frac{\pi}{3}\right), \\
-\mathrm{Ls}_3\left(\frac{\pi}{3}\right) &= \frac{7}{108}\pi^3, \\
\mathrm{Ls}_4\left(\frac{\pi}{3}\right) &= \frac{1}{2}\pi\,\zeta(3) + \frac{9}{2}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right), \\
-\mathrm{Ls}_5\left(\frac{\pi}{3}\right) &= \frac{1543}{19440}\pi^5 - 6\,\mathrm{Gl}_{4,1}\left(\frac{\pi}{3}\right), \\
\mathrm{Ls}_6\left(\frac{\pi}{3}\right) &= \frac{15}{2}\pi\,\zeta(5) + \frac{35}{36}\pi^3\zeta(3) + \frac{135}{2}\,\mathrm{Cl}_6\left(\frac{\pi}{3}\right), \\
-\mathrm{Ls}_7\left(\frac{\pi}{3}\right) &= \frac{74369}{326592}\pi^7 + \frac{15}{2}\pi\zeta(3)^2 - 135\,\mathrm{Gl}_{6,1}\left(\frac{\pi}{3}\right), \\
\mathrm{Ls}_8\left(\frac{\pi}{3}\right) &= \frac{13181}{2592}\pi^5\zeta(3) + \frac{1225}{24}\pi^3\zeta(5) + \frac{319445}{864}\pi\zeta(7) \\
&\quad + \frac{35}{2}\pi^2\,\mathrm{Cl}_6\left(\frac{\pi}{3}\right) + \frac{945}{4}\,\mathrm{Cl}_8\left(\frac{\pi}{3}\right) + 315\,\mathrm{Cl}_{6,1,1}\left(\frac{\pi}{3}\right),
\end{aligned}$$

and so forth, where we note that each integral is a multivariable rational polynomial in π as well as Cl, Gl, and zeta values.

The first presumed-irreducible value that occurs is

$$\begin{aligned}
\mathrm{Gl}_{4,1}\left(\frac{\pi}{3}\right) &= \sum_{n=1}^{\infty} \frac{\sum_{k=1}^{n-1}\frac{1}{k}}{n^4}\,\sin\left(\frac{n\pi}{3}\right) \\
&= \frac{3341}{1632960}\pi^5 - \frac{1}{\pi}\zeta(3)^2 - \frac{3}{4\pi}\sum_{n=1}^{\infty}\frac{1}{\binom{2n}{n}n^6}.
\end{aligned} \tag{6.13}$$

[1] available for download from http://arminstraub.com/pub/log-sine-integrals

The final evaluation is described in [BBK01]. Extensive computation suggests it is not reducible in the sense of Example 6.2.3. Indeed, conjectures are made in [BBK01, §5] for the number of irreducible Clausen and Glaisher values at each depth. $\diamondsuit$

Example 6.2.5 (Central binomial sums)**.** As suggested by (6.13), the log-sine integral $\mathrm{Ls}_n^{(1)}(\pi/3)$ has an appealing evaluation in terms of the central binomial sum

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

which is given by

$$-\mathrm{Ls}_{n+2}^{(1)}\left(\frac{\pi}{3}\right) = n! \left(-\frac{1}{2}\right)^n \mathcal{S}_+(n+2). \tag{6.14}$$

This is proven in [BBK01, Lemma 1], in connection with a study of Apéry-like sums — of which the value $\frac{5}{2}\mathcal{S}_-(3) = \zeta(3)$ plays a role in Apéry's proof of the later's irrationality. The story of Apéry's proof is charmingly described in Alf van der Poorten's most cited paper [Poo79].

Comtet's evaluation $\mathcal{S}_+(4) = \frac{17}{36}\zeta(4)$ thus also evaluates $\mathrm{Ls}_4^{(1)}\left(\frac{\pi}{3}\right) = -\frac{17\pi^4}{6480}$, while the classical arcsin series gives $\mathrm{Ls}_2^{(1)}\left(\frac{\pi}{3}\right) = -\frac{\pi^2}{18}$. We recall from [BBK01] that, for instance,

$$\mathcal{S}_+(8) = \frac{3462601}{2204496000}\pi^8 + \frac{1}{9}\pi^2\zeta(3)^2 - \frac{38}{3}\zeta(3)\zeta(5) - \frac{14}{15}\zeta(5,3) - 4\pi\,\mathrm{Gl}_{6,1}\left(\frac{\pi}{3}\right).$$

Thus, apart from MZVs, $\mathcal{S}_+(8)$ involves the same Clausen value $\mathrm{Gl}_{6,1}\left(\frac{\pi}{3}\right)$ as appears in $\mathrm{Ls}_7\left(\frac{\pi}{3}\right)$ (and hence $\mu_6(1+x+y_*)$). In other words, $\mu_6(1+x+y_*)$ can be written entirely in terms of MZVs and $\mathcal{S}_+(8)$. This is true for the other cases in Example 6.3.1 as well: $\mu_k(1+x+y_*)$ can be written in terms of MZVs as well as $\mathcal{S}_+(k+2)$ for $k \leqslant 6$. $\diamondsuit$

6.2.3 Generalized log-sine integrals at π

Following [BS11c], we demonstrate how the generalized log-sine integrals $\mathrm{Ls}_n^{(k)}(\pi)$ may be extracted from a generating function given in Theorem 6.2.6. As Lewin [Lew81, §7.9] sketches, at least for small values of n and k, these log-sine integrals at π have closed forms involving zeta values and Kummer-type constants such as $\mathrm{Li}_4(1/2)$. This will be made more precise in Remark 6.2.8. We start with the generating function identity

$$\begin{aligned} -\sum_{n,k\geqslant 0} \mathrm{Ls}_{n+k+1}^{(k)}(\pi)\frac{\lambda^n}{n!}\frac{(i\mu)^k}{k!} &= \int_0^\pi \left(2\sin\frac{\theta}{2}\right)^\lambda \mathrm{e}^{i\mu\theta}\,\mathrm{d}\theta \\ &= i\mathrm{e}^{i\pi\frac{\lambda}{2}}\, B\left(\mu-\frac{\lambda}{2}, 1+\lambda\right) - i\mathrm{e}^{i\pi\mu} B_{1/2}\left(\mu-\frac{\lambda}{2}, -\mu-\frac{\lambda}{2}\right) \end{aligned} \tag{6.15}$$

given in [Lew81]. Here B_x is the *incomplete Beta* function. With care — because of the singularities at zero — (6.15) can be differentiated as needed as suggested by Lewin.

Using the identities, valid for $a, b > 0$ and $0 < x < 1$,

$$B_x(a,b) = \frac{x^a(1-x)^{b-1}}{a}\,{}_2F_1\left(\left.\begin{matrix}1-b, 1\\ a+1\end{matrix}\right|\frac{x}{x-1}\right) = \frac{x^a(1-x)^b}{a}\,{}_2F_1\left(\left.\begin{matrix}a+b, 1\\ a+1\end{matrix}\right|x\right),$$

found for instance in [OLBC10, §8.17(ii)], the generating function (6.15) can be rewritten as

$$-\sum_{n,k\geqslant 0} \mathrm{Ls}_{n+k+1}^{(k)}(\pi)\frac{\lambda^n}{n!}\frac{(i\mu)^k}{k!} = i\mathrm{e}^{i\pi\frac{\lambda}{2}}\left(B_1\left(\mu-\frac{\lambda}{2}, 1+\lambda\right) - B_{-1}\left(\mu-\frac{\lambda}{2}, 1+\lambda\right)\right).$$

Upon expanding the right-hand side this establishes the following computationally more accessible form given in [BS11c]:

Theorem 6.2.6 (Generating function for $\mathrm{Ls}_{n+k+1}^{(k)}(\pi)$)**.** *For* $2|\mu| < \lambda < 1$ *we have*

$$-\sum_{n,k\geqslant 0} \mathrm{Ls}_{n+k+1}^{(k)}(\pi)\,\frac{\lambda^n}{n!}\frac{(i\mu)^k}{k!} = i\sum_{n\geqslant 0}(-1)^n\binom{\lambda}{n}\frac{\mathrm{e}^{i\pi\frac{\lambda}{2}} - (-1)^n\mathrm{e}^{i\pi\mu}}{\mu - \frac{\lambda}{2} + n}. \tag{6.16}$$

The log-sine integrals $\mathrm{Ls}_n^{(k)}(\pi)$ can be quite comfortably extracted from (6.16) by appropriately differentiating its right-hand side. For that purpose it is very helpful to observe that

$$\frac{(-1)^\alpha}{\alpha!}\left(\frac{\mathrm{d}}{\mathrm{d}\lambda}\right)^\alpha\binom{\lambda}{n}\bigg|_{\lambda=0} = \frac{(-1)^n}{n}\sum_{n>i_1>i_2>\ldots>i_{\alpha-1}}\frac{1}{i_1 i_2\cdots i_{\alpha-1}}. \tag{6.17}$$

Fuller theoretical and computational details are given in [BS11c].

The general process is now exemplified for the cases $\mathrm{Ls}_4^{(2)}(\pi)$ and $\mathrm{Ls}_5^{(1)}(\pi)$.

Example 6.2.7 ($\mathrm{Ls}_4^{(k)}(\pi)$ and $\mathrm{Ls}_5^{(k)}(\pi)$)**.** In order to find $\mathrm{Ls}_4^{(2)}(\pi)$ we differentiate (6.16) once with respect to λ and twice with respect to μ. To further simplify computation, we take advantage of the fact that the result will be real which allows us to neglect imaginary parts:

$$\begin{aligned} -\mathrm{Ls}_4^{(2)}(\pi) &= \frac{\mathrm{d}^2}{\mathrm{d}\mu^2}\frac{\mathrm{d}}{\mathrm{d}\lambda} i\sum_{n\geqslant 0}\binom{\lambda}{n}\frac{(-1)^n\mathrm{e}^{i\pi\frac{\lambda}{2}} - \mathrm{e}^{i\pi\mu}}{\mu - \frac{\lambda}{2} + n}\bigg|_{\lambda=\mu=0} \\ &= 2\pi\sum_{n\geqslant 1}\frac{(-1)^{n+1}}{n^3} = \frac{3}{2}\,\pi\zeta(3). \end{aligned} \tag{6.18}$$

In the second step we were able to drop the term corresponding to $n = 0$ because its contribution $-i\pi^4/24$ is purely imaginary.

Similarly, writing $H_{n-1}^{(1,1)} = \sum_{n>n_1>n_2} \frac{1}{n_1 n_2}$, we obtain $\mathrm{Ls}_5^{(1)}(\pi)$ as

$$\begin{aligned}
-\mathrm{Ls}_5^{(1)}(\pi) &= \frac{3}{4}\sum_{n\geqslant 1} \frac{6(1-(-1)^n)}{n^5} - \frac{\pi^2}{n^3} + \frac{8(1-(-1)^n)}{n^4}\left(nH_{n-1}^{(1,1)} - H_{n-1}\right) \\
&= \frac{9}{2}\left(\zeta(5) - \mathrm{Li}_5(-1)\right) - \frac{3}{4}\pi^2\zeta(3) \\
&+ 6\left(\mathrm{Li}_{3,1,1}(1) - \mathrm{Li}_{3,1,1}(-1) - \mathrm{Li}_{4,1}(1) + \mathrm{Li}_{4,1}(-1)\right) \\
&= 2\,\lambda_5\left(\tfrac{1}{2}\right) - \frac{3}{4}\pi^2\zeta(3) - \frac{93}{32}\zeta(5). \qquad (6.19)
\end{aligned}$$

Here λ_5 is as defined in (1.17). Further such evaluations include

$$-\mathrm{Ls}_4^{(1)}(\pi) = 2\lambda_4\left(\tfrac{1}{2}\right) - \frac{19}{8}\zeta(4), \qquad (6.20)$$

$$-\mathrm{Ls}_5^{(2)}(\pi) = 4\pi\,\lambda_4\left(\tfrac{1}{2}\right) - \frac{3}{40}\pi^5, \qquad (6.21)$$

$$-\mathrm{Ls}_5^{(3)}(\pi) = \frac{9}{4}\pi^2\zeta(3) - \frac{93}{8}\zeta(5). \qquad (6.22)$$

$\mathrm{Ls}_5^{(2)}(\pi)$ has also been evaluated in [Lew81, Eqn. (7.145)] but the exact formula was not given correctly. ♢

Remark 6.2.8. From the form of (6.16) and (6.17) we can see that the log-sine integrals $\mathrm{Ls}_n^{(k)}(\pi)$ can be expressed in terms of π and the polylogarithms $\mathrm{Li}_{n,\{1\}_m}(\pm 1)$. Further, the duality results in [BBBL01, §6.3, and Example 2.4] show that the terms $\mathrm{Li}_{n,\{1\}_m}(-1)$ will produce explicit multi-polylogarithmic values at 1/2. ♢

The next example illustrates the rapidly growing complexity of these integrals, especially when compared to the evaluations given in Example 6.2.7.

Example 6.2.9 ($\mathrm{Ls}_6^{(k)}(\pi)$ and $\mathrm{Ls}_7^{(3)}(\pi)$)**.** Proceeding as in Example 6.2.7 and writing

$$\mathrm{Li}^{\pm}_{a_1,\ldots,a_n} = \mathrm{Li}_{a_1,\ldots,a_n}(1) - \mathrm{Li}_{a_1,\ldots,a_n}(-1)$$

we find

$$
\begin{aligned}
-\operatorname{Ls}_6^{(1)}(\pi) &= -24\operatorname{Li}^{\pm}_{3,1,1,1} + 24\operatorname{Li}^{\pm}_{4,1,1} - 18\operatorname{Li}^{\pm}_{5,1} + 12\operatorname{Li}^{\pm}_{6} + 3\pi^2\zeta(3,1) - 3\pi^2\zeta(4) + \frac{\pi^6}{480} \\
&= \frac{43}{60}\log^6 2 - \frac{7}{12}\pi^2\log^4 2 + 9\zeta(3)\log^3 2 + \left(24\operatorname{Li}_4\left(\tfrac{1}{2}\right) - \frac{1}{120}\pi^4\right)\log^2 2 \\
&\quad + \left(36\operatorname{Li}_5\left(\tfrac{1}{2}\right) - \pi^2\zeta(3)\right)\log 2 + 12\operatorname{Li}_{5,1}\left(\tfrac{1}{2}\right) + 24\operatorname{Li}_6\left(\tfrac{1}{2}\right) - \frac{247}{10080}\pi^6 \\
&= 2\lambda_6\left(\tfrac{1}{2}\right) - 6\operatorname{Li}_{5,1}(-1) - 3\zeta(3)^2 - \frac{451}{10080}\pi^6. \qquad (6.23)
\end{aligned}
$$

In the first equality, the term $\pi^6/480$ is the one corresponding to $n = 0$ in (6.16). Similarly, we find

$$-\operatorname{Ls}_6^{(2)}(\pi) = 4\pi\lambda_5\left(\tfrac{1}{2}\right) - \pi^3\zeta(3) - \frac{189}{16}\pi\zeta(5), \qquad (6.24)$$

$$-\operatorname{Ls}_6^{(3)}(\pi) = 6\pi^2\lambda_4\left(\tfrac{1}{2}\right) - 12\operatorname{Li}_{5,1}(-1) - 6\zeta(3)^2 - \frac{187}{1680}\pi^6, \qquad (6.25)$$

$$-\operatorname{Ls}_6^{(4)}(\pi) = -\frac{45}{2}\pi\zeta(5) + 3\pi^3\zeta(3), \qquad (6.26)$$

as well as

$$
\begin{aligned}
-\operatorname{Ls}_7^{(3)}(\pi) &= \frac{9}{35}\log^7 2 + \frac{4}{5}\pi^2\log^5 2 + 9\zeta(3)\log^4 2 - \frac{31}{30}\pi^4\log^3 2 \\
&\quad - \left(72\operatorname{Li}_5\left(\tfrac{1}{2}\right) - \frac{9}{8}\zeta(5) - \frac{51}{4}\pi^2\zeta(3)\right)\log^2 2 \\
&\quad + \left(72\operatorname{Li}_{5,1}\left(\tfrac{1}{2}\right) - 216\operatorname{Li}_6\left(\tfrac{1}{2}\right) + 36\pi^2\operatorname{Li}_4\left(\tfrac{1}{2}\right)\right)\log 2 + 72\operatorname{Li}_{6,1}\left(\tfrac{1}{2}\right) \\
&\quad - 216\operatorname{Li}_7\left(\tfrac{1}{2}\right) + 36\pi^2\operatorname{Li}_5\left(\tfrac{1}{2}\right) - \frac{1161}{32}\zeta(7) - \frac{375}{32}\pi^2\zeta(5) + \frac{1}{10}\pi^4\zeta(3) \\
&= 6\pi^2\lambda_5\left(\tfrac{1}{2}\right) + 36\operatorname{Li}_{5,1,1}(-1) - \pi^4\zeta(3) - \frac{759}{32}\pi^2\zeta(5) - \frac{45}{32}\zeta(7). \qquad (6.27)
\end{aligned}
$$

Note that in each case the monomials in $\operatorname{Ls}_n^{(k)}(\pi)$ are of total order n — where π is order one, $\zeta(3)$ is order three and so on. ◊

Remark 6.2.10. A purely real form of Theorem 6.2.6 is the following:

$$\int_0^\pi \left(2\sin\frac{\theta}{2}\right)^x \mathrm{e}^{\theta y} d\theta = \sum_{n=0}^\infty \frac{(-1)^n \binom{x}{n} \left(y\left((-1)^n \mathrm{e}^{\pi y} - \cos\frac{\pi x}{2}\right) - \left(n-\frac{x}{2}\right)\sin\frac{\pi x}{2}\right)}{\left(n-\frac{x}{2}\right)^2 + y^2}. \tag{6.28}$$

One may now also deduce one-variable generating functions from (6.28). For instance,

$$\sum_{n=0}^\infty \mathrm{Ls}_{n+2}^{(1)}(\pi)\frac{\lambda^n}{n!} = \sum_{n=0}^\infty \binom{\lambda}{n} \frac{(-1)^n \cos\frac{\pi\lambda}{2} - 1}{\left(n-\frac{\lambda}{2}\right)^2}, \tag{6.29}$$

and we may again now extract individual values. ♢

6.2.4 Hypergeometric evaluation of $\mathrm{Ls}_n(\pi/3)$

We close this section with an alternative approach to the evaluation of $\mathrm{Ls}_n(\pi/3)$ complementing the one given in Section 6.2.2.

Theorem 6.2.11 (Hypergeometric form of $\mathrm{Ls}_n\left(\frac{\pi}{3}\right)$)**.** *For nonnegative integers n,*

$$\frac{(-1)^{n+1}}{n!}\mathrm{Ls}_{n+1}\left(\frac{\pi}{3}\right) = {}_{n+2}F_{n+1}\left(\left.\begin{matrix}\left\{\frac{1}{2}\right\}^{n+2} \\ \left\{\frac{3}{2}\right\}^{n+1}\end{matrix}\right| \frac{1}{4}\right) = \sum_{k=0}^\infty \frac{2^{-4k}}{(2k+1)^{n+1}}\binom{2k}{k}. \tag{6.30}$$

Consequently,

$$-\sum_{n=0}^\infty \mathrm{Ls}_{n+1}\left(\frac{\pi}{3}\right)\frac{s^n}{n!} = \frac{1}{s+1}\,{}_2F_1\left(\left.\begin{matrix}\frac{1}{2}, \frac{s}{2}+\frac{1}{2} \\ \frac{s}{2}+\frac{3}{2}\end{matrix}\right| \frac{1}{4}\right) = \sum_{k=0}^\infty \frac{2^{-4k}}{2k+1+s}\binom{2k}{k}.$$

Proof. We compute as follows:

$$\begin{aligned}
-\mathrm{Ls}_{n+1}\left(\frac{\pi}{3}\right) &= \int_0^{\pi/3} \log^n\left(2\sin\frac{\theta}{2}\right)\mathrm{d}\theta \\
&= \int_0^1 \frac{\log^n(x)}{\sqrt{1-x^2/4}}\,\mathrm{d}x \\
&= \sum_{k=0}^\infty 2^{-4k}\binom{2k}{k}\int_0^1 x^{2k}\log^n(x)\,\mathrm{d}x.
\end{aligned}$$

The claim thus follows from

$$\int_0^1 x^{s-1}\log^n(x)\,\mathrm{d}x = \int_0^\infty (-x)^n e^{-sx}\,\mathrm{d}x = \frac{(-1)^n\Gamma(n+1)}{s^{n+1}}$$

which is a consequence of the integral representation of the gamma function. □

Observe that the sum in (6.30) converges very rapidly and so is very suitable for computation. Also, from Example 6.2.4 we have evaluations — some known — such as

$$\sum_{k=0}^\infty \frac{2^{-4k}}{(2k+1)}\binom{2k}{k} = \frac{\pi}{3}$$

and

$$\sum_{k=0}^\infty \frac{2^{-4k}}{(2k+1)^2}\binom{2k}{k} = \mathrm{Cl}_2\left(\frac{\pi}{3}\right).$$

Remark 6.2.12. As outlined in [DK01], the series (6.30) combined with (6.14) can also be used to produce rapidly-convergent series for certain multi zeta values including $\zeta(5,3)$, $\zeta(7,3)$ and $\zeta(3,5,3)$. ◊

6.3 Log-sine evaluations of multiple Mahler measures

We first substantiate that we can recursively determine $\mu_k(1+x+y_*)$ from equation (6.10) as claimed.

6.3.1 Evaluation of $\mu_k(1+x+y_*)$

Substituting the values given in Example 6.2.4 and Example 6.2.2 into equation (6.10) we obtain the following multiple Mahler evaluations:

Example 6.3.1 (Values of $\mu_k(1+x+y_*)$)**.** We have

$$\mu_1(1+x+y_*) = \frac{1}{\pi}\operatorname{Cl}_2\left(\frac{\pi}{3}\right), \tag{6.31}$$
$$\mu_2(1+x+y_*) = \frac{\pi^2}{54}, \tag{6.32}$$
$$\mu_3(1+x+y_*) = \frac{9}{2\pi}\operatorname{Cl}_4\left(\frac{\pi}{3}\right) - \zeta(3), \tag{6.33}$$
$$\mu_4(1+x+y_*) = \frac{6}{\pi}\operatorname{Gl}_{4,1}\left(\frac{\pi}{3}\right) - \frac{\pi^4}{4860}, \tag{6.34}$$
$$\mu_5(1+x+y_*) = \frac{135}{2\pi}\operatorname{Cl}_6\left(\frac{\pi}{3}\right) - 15\zeta(5) - \frac{5}{18}\pi^2\zeta(3), \tag{6.35}$$
$$\mu_6(1+x+y_*) = \frac{135}{\pi}\operatorname{Gl}_{6,1}\left(\frac{\pi}{3}\right) + 15\zeta(3)^2 - \frac{943}{40824}\pi^6, \tag{6.36}$$

and the like. The first is again a form of Smyth's result (6.5). ◊

Remark 6.3.2. Note that we may rewrite the multiple Mahler measure $\mu_k(1+x+y_*)$ as follows:

$$\mu_k(1+x+y_*) = \mu(\underbrace{1+x,\ldots,1+x}_{k-1}, 1+x+y). \tag{6.37}$$

This is easily seen from Jensen's formula (6.4). Indeed, using (6.4) the left-hand side of (6.37) becomes

$$\begin{aligned}
\mu_k(1+x+y_*) &= \int_0^1 \cdots \int_0^1 \prod_{j=1}^{k} \log\left|1+e^{2\pi i s}+e^{2\pi i t_j}\right| \mathrm{d}s\mathrm{d}t_1\cdots\mathrm{d}t_k \\
&= \int_0^1 \left[\int_0^1 \log\left|1+e^{2\pi i s}+e^{2\pi i t}\right| \mathrm{d}t\right]^k \mathrm{d}s \\
&= \int \log^k\left|1+e^{2\pi i s}\right| \mathrm{d}s
\end{aligned}$$

where the last integral is over $0 \leqslant s \leqslant 1$ such that $|1+e^{2\pi i s}| \geqslant 1$. The same integral is obtained when applying (6.4) to the right-hand side of (6.37). ◊

6.3.2 Evaluation of $\mu_k(1+x+y_*+z_*)$

We next follow a similar course for multiple Mahler measures built from $1+x+y+z$ to that given for $\mu_k(1+x+y_*)$ in Section 6.3.1. Analogous to (6.8) we define:

$$\mu_k(1+x+y_*+z_*) := \mu(1+x+y_1+z_1,\ldots,1+x+y_k+z_k). \tag{6.38}$$

Working as in (6.7) we may write

$$\mu_k(1+x+y_*+z_*) = \frac{1}{\pi}\int_0^\pi \left[\frac{1}{\pi}\int_0^\pi \max\left\{\log\left(2\sin\frac{\theta}{2}\right),\log\left(2\sin\frac{\sigma}{2}\right)\right\}\,\mathrm{d}\sigma\right]^k \mathrm{d}\theta.$$

We observe that the inner integral with respect to σ evaluates separately, and on recalling that $\mathrm{Ls}_2(\theta) = \mathrm{Cl}_2(\theta)$ and $\mathrm{Cl}_2(\pi) = 0$ we arrive at:

Theorem 6.3.3. *For all positive integers k, we have*

$$\mu_k(1+x+y_*+z_*) = \frac{1}{\pi^{k+1}}\int_0^\pi \left(\theta\log\left(2\sin\frac{\theta}{2}\right)+\mathrm{Cl}_2(\theta)\right)^k \mathrm{d}\theta. \tag{6.39}$$

Example 6.3.4 (Values of $\mu_k(1+x+y_*+z_*)$)**.** Thus, for $\mu_2(1+x+y_*+z_*)$, we obtain

$$\pi^3\,\mu_2(1+x+y_*+z_*) = -\mathrm{Ls}_5^{(2)}(\pi) + \int_0^\pi \mathrm{Cl}_2^2(\theta)\,\mathrm{d}\theta + \int_0^\pi 2\theta\,\log\left(2\,\sin\frac{\theta}{2}\right)\,\mathrm{Cl}_2(\theta)\,\mathrm{d}\theta.$$

Applying Parseval's equation evaluates the first integral in this equation to $\pi^5/180$. Integration by parts of the second integral shows that it equals minus the first one.

For $k = 3$, one term is a log-sine integral and two of the terms are equal, but we could not completely evaluate the two remaining terms.

Hence, from (6.39), we have:

$$\mu_1(1+x+y_*+z_*) = -\frac{2}{\pi^2}\,\mathrm{Ls}_3^{(1)}(\pi) = \frac{7}{2}\frac{\zeta(3)}{\pi^2}, \tag{6.40}$$

$$\mu_2(1+x+y_*+z_*) = -\frac{1}{\pi^3}\,\mathrm{Ls}_5^{(2)}(\pi) + \frac{\pi^2}{90} = \frac{4}{\pi^2}\,\mathrm{Li}_{3,1}(-1) + \frac{7}{360}\pi^2, \tag{6.41}$$

$$\mu_3(1+x+y_*+z_*) = \frac{2}{\pi^4}\int_0^\pi \mathrm{Cl}_2^3(\theta)\,\mathrm{d}\theta + \frac{3}{\pi^4}\int_0^\pi \theta^2\log^2\left(2\sin\frac{\theta}{2}\right)\mathrm{Cl}_2(\theta)\,\mathrm{d}\theta - \frac{1}{\pi^4}\,\mathrm{Ls}_7^{(3)}(\pi)\,. \tag{6.42}$$

The first of these is a form of (6.7) which originates with Smyth and Boyd [Boy81]. The relevant log-sine integrals have been discussed in Section 6.2.3. In particular, $\mathrm{Ls}_5^{(2)}(\pi)$ and $\mathrm{Ls}_7^{(3)}(\pi)$ have been evaluated in (6.21) and (6.27).

It is possible to further reexpress the integrals in (6.42) but we have not so far found an entirely satisfactory resolution. ♢

6.3.3 Evaluation of $\mu(1+x,\ldots,1+x,1+x+y+z)$

Recall from Remark 6.3.2 that the multiple Mahler measure $\mu_k(1+x+y_*)$ can be rewritten as $\mu(1+x,\ldots,1+x,1+x+y)$ with the term $1+x$ repeated $k-1$ times. This is not possible for $\mu_k(1+x+y_*+z_*)$ which is distinct from $\mu(1+x,\ldots,1+x,1+x+y+z)$ which we study next.

Applying Jensen's formula as in (6.7) for $k=0,1,2,\ldots$ we obtain (6.43) below. Then (6.44) follows on integrating by parts.

Theorem 6.3.5. *For all nonnegative integers k we have:*

$$\mu(\underbrace{1+x,\ldots,1+x}_{k},1+x+y+z)$$

$$= -\frac{1}{\pi^2}\,\mathrm{Ls}_{k+3}^{(1)}(\pi) + \frac{1}{\pi^2}\int_0^\pi \mathrm{Ls}_2(\theta)\log^k\left(2\sin\frac{\theta}{2}\right)\mathrm{d}\theta \tag{6.43}$$

$$= -\frac{1}{\pi^2}\,\mathrm{Ls}_{k+3}^{(1)}(\pi) - \frac{1}{\pi^2}\int_0^\pi \mathrm{Ls}_{k+1}(\theta)\log\left(2\sin\frac{\theta}{2}\right)\mathrm{d}\theta. \tag{6.44}$$

Example 6.3.6. Equation (6.44) recovers (6.7) when $k = 0$ since $\mathrm{Ls}_1(\theta) = -\theta$. Setting $k = 1$ in (6.44) we obtain

$$\begin{aligned}
\mu(1+x, 1+x+y+z) &= -\frac{1}{\pi^2}\,\mathrm{Ls}_4^{(1)}(\pi) + \frac{1}{\pi^2}\int_0^\pi \mathrm{Cl}_2(\theta)\,\log\left(2\sin\frac{\theta}{2}\right)\,\mathrm{d}\theta \\
&= -\frac{1}{\pi^2}\,\mathrm{Ls}_4^{(1)}(\pi) - \frac{1}{2\pi^2}\,\mathrm{Cl}_2^2(\pi) \\
&= -\frac{1}{\pi^2}\,\mathrm{Ls}_4^{(1)}(\pi) = \frac{2}{\pi^2}\lambda_4\left(\tfrac{1}{2}\right) - \frac{19}{720}\pi^2
\end{aligned} \tag{6.45}$$

on again using $\mathrm{Ls}_2(\theta) = \mathrm{Cl}_2(\theta)$ and $\mathrm{Cl}_2(\pi) = 0$. The final evaluation was given in (6.20) of Example 6.2.7. For $k = 2$ we have

$$\begin{aligned}
\mu(1+x, 1+x, 1+x+y+z) &= -\frac{1}{\pi^2}\,\mathrm{Ls}_5^{(1)}(\pi) + \frac{1}{\pi^2}\int_0^\pi \mathrm{Ls}_2(\theta)\log^2\left(2\sin\frac{\theta}{2}\right)\,\mathrm{d}\theta \\
&= -\frac{1}{\pi^2}\,\mathrm{Ls}_5^{(1)}(\pi) - \frac{2}{3\pi^2}\lambda_5\left(\tfrac{1}{2}\right) + \frac{155}{32\pi^2}\,\zeta(5),
\end{aligned}$$

where the last integral was found via PSLQ. This agrees with the more complicated version conjectured in [Kal05]. We may use (6.19) of Example 6.2.7 to arrive at

$$\mu(1+x, 1+x, 1+x+y+z) = \frac{4}{3\pi^2}\lambda_5\left(\tfrac{1}{2}\right) - \frac{3}{4}\zeta(3) + \frac{31}{16\pi^2}\zeta(5). \tag{6.46}$$

For $k = 3$, things are more complicated as is suggested by (6.23). ♢

6.4 Moments of random walks

The s-th moments of an n-step uniform random walk are given by

$$W_n(s) = \int_0^1 \cdots \int_0^1 \left|\sum_{k=1}^n e^{2\pi i t_k}\right|^s \mathrm{d}t_1 \cdots \mathrm{d}t_n \tag{6.47}$$

and their relation with Mahler measure is observed in [BSWZ11]. In particular,

$$W_n'(0) = \mu(1 + x_1 + \ldots + x_{n-1})$$

with the cases $n = 3$ and $n = 4$ given in (6.5) and (6.7) respectively. The cases $n = 5$ and $n = 6$ are discussed in (6.75) and (6.76) respectively. Higher derivatives of W_n correspond to higher Mahler measures:

$$W_n^{(k)}(0) = \mu_k(1 + x_1 + \ldots + x_{n-1}). \tag{6.48}$$

More general moments corresponding to other Mahler measures were introduced in [Aka09] and studied in [KLO08] as *zeta Mahler measures*.

6.4.1 Evaluation of $\mu_k(1 + x)$

Equipped with the results of the first section, we may now fruitfully revisit another recent result which is concerned with the evaluation of $W_2^{(k)}(0) = \mu_k(1 + x)$.

A central evaluation in [KLO08, Thm. 3] is:

$$\mu_k(1 + x) = (-1)^k k! \sum_{n=1}^{\infty} \frac{1}{4^n} \sum_{b_j \geqslant 2, \sum b_j = k} \zeta(b_1, b_2, \ldots, b_n). \tag{6.49}$$

We note that directly from the definition and an easy change of variables

$$\mu_k(1 + x) = -\frac{1}{\pi} \operatorname{Ls}_{k+1}(\pi). \tag{6.50}$$

Hence, we have closed forms such as provided by Example 6.2.2.

Example 6.4.1. For instance,

$$-\mu_5(1+x) = \frac{45}{2}\zeta(5) + \frac{5}{4}\pi^2\zeta(3), \tag{6.51}$$

$$\mu_6(1+x) = \frac{45}{2}\zeta^2(3) + \frac{275}{1344}\pi^6. \tag{6.52}$$

These are derived more elaborately in [KLO08, Ex. 5] from the right of equation (6.49). $\diamondsuit$

We have, inter alia, evaluated the multi zeta value sum on the right of equation (6.49) as a simple log-sine integral.

Also, note that the evaluation $W_2(s) = \binom{s}{s/2}$, [BSWZ11], in combination with (6.50) thus explains and proves the generating function (6.12).

6.4.2 A generating function for $\mu_k(1+x+y)$

The evaluation of the Mahler measures $W_3'(0) = \mu(1+x+y)$ and $W_4'(0) = \mu(1+x+y+z)$ is classical and was discussed in Example 6.1.2.

The derivatives $W_3''(0) = \mu_2(1+x+y)$ and $W_4''(0) = \mu_2(1+x+y+z)$ were evaluated using explicit forms for $W_3(s)$ and $W_4(s)$ in [BSWZ11, §6]. For example,

$$W_3''(0) = \frac{\pi^2}{12} - \frac{4\log 2}{\pi}\operatorname{Cl}_2\left(\frac{\pi}{3}\right) - \frac{4}{\pi}\sum_{n=0}^{\infty}\frac{\binom{2n}{n}}{4^{2n}}\frac{\sum_{k=0}^{n}\frac{1}{2k+1}}{(2n+1)^2}. \tag{6.53}$$

We shall revisit these two Mahler measures in (6.58) and (6.73) of Sections 6.4.3 and 6.4.4.

As a consequence of the study of random walks in [BSWZ11] we record the following generating function for $\mu_k(1+x+y)$ which follows from (6.48) and the hypergeometric expression for W_3 in [BSWZ11, Thm. 10]. There is a corresponding expression, using a single Meijer-G function, for W_4 (i.e., $\mu_m(1+x+y+z)$) given in [BSWZ11, Thm. 11].

Theorem 6.4.2. *For complex $|s|<2$, we may write*

$$\sum_{m=0}^{\infty} \mu_m(1+x+y)\frac{s^m}{m!} = W_3(s) = \frac{\sqrt{3}}{2\pi}\, 3^{s+1}\, \frac{\Gamma(1+s/2)^2}{\Gamma(s+2)}\, {}_3F_2\left({\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2} \atop 1, \frac{s+3}{2}} \middle| \frac{1}{4} \right). \quad (6.54)$$

The particular measure $\mu_2(1+x+y)$ will be investigated in Section 6.4.3. The general case $\mu_m(1+x+y)$ is studied in [BBSW12].

6.4.3 Evaluation of $\mu_2(1+x+y)$

Example 6.4.3. A purported evaluation given in [KLO08] is:

$$\mu_2(1+x+y) = \mu_2(1+x+y) \overset{?}{=} \frac{5}{54}\pi^2 = 5\mu_2(1+x+y_*) \quad (6.55)$$

where the last equality follows from (6.32). However, we are able to numerically disprove (6.55).[2] Indeed, we find $\mu_2(1+x+y) \approx 0.419299$ while $\frac{5}{54}\pi^2 \approx 0.913852$. $\diamondsuit$

We note that for integer $k \geqslant 1$ we do have

$$\mu_k(1+x+y) = \frac{1}{4\pi^2}\int_0^{2\pi} \mathrm{d}\theta \int_0^{2\pi} \left(\mathrm{Re}\,\log\left(1-2\sin(\theta)\mathrm{e}^{i\omega}\right)\right)^k \mathrm{d}\omega, \quad (6.56)$$

directly from the definition and some simple trigonometry, since Re log $=\log|\cdot|$. We revisit Example 6.4.3 in the next result, in which we evaluate $\mu_2(1+x+y)$ as a log-sine integrals as well as in terms of polylogarithmic constants.

[2]There are two errors in the proof given in [KLO08, Theorem 11]. A term is dropped between lines 8 and 9 of the proof and the limits of integration are wrong after changing $s(1-s)$ to t.

Theorem 6.4.4. *We have*

$$\mu_2(1+x+y) = \frac{24}{5\pi}\,\mathrm{Ti}_3\left(\frac{1}{\sqrt{3}}\right) + \frac{2\log 3}{\pi}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) - \frac{\log^2 3}{10} - \frac{19\pi^2}{180} \tag{6.57}$$

$$= \frac{\pi^2}{4} + \frac{3}{\pi}\,\mathrm{Ls}_3\left(\frac{2\pi}{3}\right). \tag{6.58}$$

Remark 6.4.5. We note that

$$\mathrm{Ls}_3\left(\frac{2\pi}{3}\right) = -\int_0^{\pi/3} \log^2\left(2\cos\frac{\theta}{2}\right)\,\mathrm{d}\theta$$

and that these log-cosine integrals have fewer explicit closed forms. Using the results of [BS11c] to evaluate log-sine integrals in polylogarithmic terms we find that

$$\mathrm{Ls}_3\left(\frac{2\pi}{3}\right) = -\frac{13}{162}\pi^3 - 2\,\mathrm{Gl}_{2,1}\left(\frac{2\pi}{3}\right). \tag{6.59}$$

In fact, this is automatic if we employ the provided implementation. Theorem 6.4.4 thus also gives a reduction of $\mathrm{Gl}_{2,1}\left(\frac{2\pi}{3}\right)$ to one-dimensional polylogarithmic constants.

◊

A preparatory result is helpful before proceeding to the proof of Theorem 6.4.4.

Proposition 6.4.6 (A dilogarithmic representation)**.** *We have:*

(a)

$$\frac{2}{\pi}\int_0^{\pi} \mathrm{Re}\ \mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta = 2\zeta(2). \tag{6.60}$$

(b)

$$\mu_2(1+x+y) = \frac{1}{36}\pi^2 + \frac{2}{\pi}\int_0^{\pi/6} \mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta. \tag{6.61}$$

Proof. For (a) we define $\tau(z) := \frac{2}{\pi}\int_0^{\pi} \mathrm{Li}_2\left(4z\sin^2\theta\right)\mathrm{d}\theta$. This is an analytic function of z. For $|z| < 1/4$ we may use the original series for Li_2 and expand term by term using Wallis' formula to derive

$$\begin{aligned}\tau(z) &= \frac{2}{\pi}\sum_{n\geqslant 1}\frac{(4z)^n}{n^2}\int_0^\pi \sin^{2n}\theta\,\mathrm{d}\theta = 4z\,{}_4F_3\left(\left.{1,1,1,\frac{3}{2} \atop 2,2,2}\right|4z\right)\\ &= 4\,\mathrm{Li}_2\left(\frac{1}{2}-\frac{1}{2}\sqrt{1-4z}\right) - 2\log\left(\frac{1}{2}+\frac{1}{2}\sqrt{1-4z}\right)^2.\end{aligned}$$

The final equality can be obtained in *Mathematica* and then verified by differentiation. In particular, the final function provides an analytic continuation and so we obtain $\tau(1) = 2\zeta(2) + 4i\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)$ which yields the assertion.

For (b), commencing much as in [KLO08, Thm. 11], we write

$$\mu_2(1+x+y) = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\mathrm{Re}\,\log\left(1-2\sin(\theta)\mathrm{e}^{i\,\omega}\right)^2\,\mathrm{d}\omega\,\mathrm{d}\theta.$$

We consider the inner integral $\rho(\alpha) := \int_{-\pi}^{\pi}\left(\mathrm{Re}\,\log\left(1-\alpha\,\mathrm{e}^{i\,\omega}\right)\right)^2\,\mathrm{d}\omega$ with $\alpha := 2\sin\theta$. For $|\theta| \leqslant \pi/6$ we directly apply Parseval's identity to obtain

$$\rho(2\sin\theta) = \pi\,\mathrm{Li}_2\left(4\sin^2\theta\right). \tag{6.62}$$

In the remaining case we write

$$\begin{aligned}\rho(2\sin\theta) &= \int_{-\pi}^{\pi}\left\{\log|\alpha| + \mathrm{Re}\,\log\left(1-\alpha^{-1}\,\mathrm{e}^{i\,\omega}\right)\right\}^2\,\mathrm{d}\omega\\ &= 2\pi\,\log^2|\alpha| - 2\log|\alpha|\int_{-\pi}^{\pi}\log\left|1-\alpha^{-1}\,\mathrm{e}^{i\,\omega}\right|\,\mathrm{d}\omega + \pi\,\mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\\ &= 2\pi\,\log^2|2\sin\theta| + \pi\,\mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right),\end{aligned} \tag{6.63}$$

where we have appealed to Parseval's and Jensen's formulas. Thus,

$$\mu_2(1+x+y) = \frac{1}{\pi}\int_0^{\pi/6}\mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta + \frac{1}{\pi}\int_{\pi/6}^{\pi/2}\mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\mathrm{d}\theta + \frac{\pi^2}{54}, \tag{6.64}$$

since $\frac{2}{\pi}\int_{\pi/6}^{\pi/2}\log^2\alpha\,\mathrm{d}\theta = \mu_2(1+x+y_*) = \frac{\pi^2}{54}$. Now, for $\alpha > 1$, the functional equation in [Lew58, A2.1 (6)] — $\mathrm{Li}_2(\alpha)+\mathrm{Li}_2(1/\alpha)+\frac{1}{2}\log^2\alpha = 2\zeta(2)+i\pi\log\alpha$ — gives:

$$\int_{\pi/6}^{\pi/2}\left\{\mathrm{Re}\ \mathrm{Li}_2\left(4\sin^2\theta\right)+\mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\right\}\mathrm{d}\theta = \frac{5}{54}\pi^3. \tag{6.65}$$

We now combine (6.60), (6.65) and (6.64) to deduce the desired result in (6.61). ☐

We are now in a position to prove the desired evaluation of $\mu_2(1+x+y)$ as a log-sine integral.

Proof of Theorem 6.4.4. Using Proposition 6.4.6 we have:

$$\begin{aligned}\mu_2(1+x+y) &= \frac{\pi^2}{36}+\frac{2}{\pi}\int_0^{\pi/6}\mathrm{Li}_2\left(4\,\sin^2 w\right)\,\mathrm{d}w\\ &= \frac{\pi^2}{36}+\frac{2}{\pi}\sum_{n\geqslant 1}\frac{4^n}{n^2}\int_0^{\pi/6}\sin^{2n}w\,\mathrm{d}w\\ &= \frac{\pi^2}{36}+\frac{\sqrt{3}}{\pi}\sum_{n\geqslant 1}\frac{\binom{2n-1}{n-1}}{4^n}\sum_{k=n}^{\infty}\frac{1}{(2\,k+1)\binom{2k}{k}},\end{aligned} \tag{6.66}$$

where the last line is a consequence of the formula

$$\int_0^{\pi/6}\sin^{2n}w\,\mathrm{d}w = \frac{\sqrt{3}}{2}\frac{\binom{2n-1}{n-1}}{4^n}\sum_{k=n}^{\infty}\frac{1}{(2\,k+1)\binom{2k}{k}}$$

given in [KLO08]. Hence, on using a beta-integral and then exchanging sum and integral we obtain:

$$\begin{aligned}\mu_2(1+x+y) &= \frac{\pi^2}{36}+\frac{2\sqrt{3}}{\pi}\sum_{n\geqslant 1}\binom{2n-1}{n-1}\int_0^{1/2}\frac{t^n(1-t)^n}{1-t+t^2}\,\mathrm{d}t\\ &= \frac{\pi^2}{36}+\frac{2\sqrt{3}}{\pi}\int_0^{1/2}\sum_{n\geqslant 1}\binom{2n-1}{n-1}\frac{(t(1-t))^n}{1-t+t^2}\,\mathrm{d}t\\ &= \frac{\pi^2}{36}+\frac{\sqrt{3}}{\pi}\int_0^{1/2}\frac{2\,\mathrm{Li}_2\,(t)-\log^2(1-t)}{1-t+t^2}\,\mathrm{d}t\end{aligned} \tag{6.67}$$

where the last equality comes from evaluating the power series above.

Further careful integrations by parts let us use [Lew81, Appendix A5.3, (1)] to derive

$$\pi\mu_2(1+x+y) = \frac{67}{324}\,\pi^3 + 2\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)\log 3 - 8\ \mathrm{Im}\ \mathrm{Li}_3\left(i\sqrt{3}\right) + 4\,\mathrm{Im}\ \mathrm{Li}_3\left(\frac{3+i\sqrt{3}}{2}\right). \tag{6.68}$$

Next, we note that

$$\mathrm{Im}\ \mathrm{Li}_3\left(\frac{3+i\sqrt{3}}{2}\right) = \frac{55}{1296}\,\pi^3 + \frac{5}{48}\,\pi\,\log^2 3 + \mathrm{Im}\ \mathrm{Li}_3\left(\frac{3-i\sqrt{3}}{6}\right), \tag{6.69}$$

while

$$\mathrm{Im}\ \mathrm{Li}_3\left(i\sqrt{3}\right) = \frac{1}{16}\,\pi^3 + \frac{1}{16}\,\pi\,\log^2 3 - \frac{1}{6}\ \mathrm{Ti}_3\left(\frac{1}{\sqrt{3}}\right). \tag{6.70}$$

Above, we have had recourse to various reduction formulae [Lew81, BCC10] for higher Clausen functions to arrive at the final form. Substituting (6.69), (6.70) in (6.68), we arrive at the asserted result (6.57).

A connection with the log-sine integrals is made by noting that

$$\mathrm{Ti}_3\left(\frac{1}{\sqrt{3}}\right) = \frac{5}{8}\,\mathrm{Ls}_3\left(\frac{2\pi}{3}\right) - \frac{1}{2}\ \mathrm{Ti}_2\left(\frac{1}{\sqrt{3}}\right)\log 3 - \frac{1}{48}\,\pi\,\log^2 3 + \frac{2}{27}\,\pi^3, \tag{6.71}$$

$$\mathrm{Ti}_2\left(\frac{1}{\sqrt{3}}\right) = \frac{5}{6}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) - \frac{\pi}{12}\,\log 3. \tag{6.72}$$

These follow from [Lew81, Eqn. (44), p. 298] and [Lew81, Eqn. (18), p. 292] respectively. Applying (6.71) and (6.72) to (6.57) now yields (6.58). □

Finally, we observe that it is possible to take the analysis of $\mu_n(1+x+y)$ for $n \geqslant 3$ a fair distance. This will be detailed in the forthcoming paper [BBSW12].

6.4.4 Evaluation of $\mu_2(1+x+y+z)$

Paralleling the evaluation of $\mu_2(1+x+y)$ in Theorem 6.4.4 we now give a closed form for $\mu_2(1+x+y+z)$ which was obtained in [BSWZ11] by quite different methods to those of Theorem 6.4.4.

Theorem 6.4.7. *We have*

$$\mu_2(1+x+y+z) = \frac{12}{\pi^2}\lambda_4\left(\tfrac{1}{2}\right) - \frac{\pi^2}{5} \tag{6.73}$$

where λ_4 is as defined in (1.17)*.*

Proof. The formula

$$\pi^2 W_4''(0) = 24\,\mathrm{Li}_4(\tfrac{1}{2}) - 18\zeta(4) + 21\zeta(3)\log 2 - 6\zeta(2)\log^2 2 + \log^4 2$$

was deduced in [BSWZ11]. We now observe that

$$\begin{aligned} 24\,\mathrm{Li}_4(\tfrac{1}{2}) - 18\zeta(4) + 21\zeta(3)\log 2 - 6\zeta(2)\log^2 2 + \log^4 2 \\ = 12\lambda_4\left(\tfrac{1}{2}\right) - \frac{\pi^4}{5}, \end{aligned}$$

and appeal to equation (6.48) for $\mu_2(1+x+y+z) = W_4''(0)$. ∎

6.4.5 A conjecture of Rodriguez-Villegas

Finally, we mention two conjectures concerning the Mahler measures $\mu(1+x+y+z+w)$ and $\mu(1+x+y+z+w+v)$, contained in slightly different form in [Fin05]. These correspond to the moment values $W_5'(0)$ and $W_6'(0)$.

Recall that η is the *Dirichlet eta-function* given by

$$\eta(\tau) = \eta(q) := q^{1/24} \prod_{n=1}^{\infty}(1-q^n) = q^{1/24} \sum_{n=-\infty}^{\infty} (-1)^n q^{n(3n+1)/2} \tag{6.74}$$

where $q = e^{2\pi i \tau}$.

The following two conjectural expressions have been put forth by Rodriguez-Villegas:

$$\mu(1+x+y+z+w) \stackrel{?}{=} \left(\frac{15}{4\pi^2}\right)^{5/2} \int_0^{\infty} \left\{\eta^3(e^{-3t})\eta^3(e^{-5t}) + \eta^3(e^{-t})\eta^3(e^{-15t})\right\} t^3 \,\mathrm{d}t \tag{6.75}$$

and

$$\mu(1+x+y+z+w+v) \stackrel{?}{=} \left(\frac{3}{\pi^2}\right)^{3} \int_0^{\infty} \eta^2(e^{-t})\eta^2(e^{-2t})\eta^2(e^{-3t})\eta^2(e^{-6t})\, t^4 \,\mathrm{d}t. \tag{6.76}$$

As discussed in [BSWZ11], we have confirmed numerically that the evaluation of $\mu(1+x+y+z+w+v)$ in (6.75) holds to 600 places. Likewise, we have confirmed that (6.76) holds to 80 places.

6.5 Conclusion

It is reasonable to ask what other Mahler measures can be placed in log-sine form, and to speculate as to whether the η integrals (6.75) and (6.76) can be.

As described in [LS11], it is a long standing question due to Lehmer as to whether, for single-variable integer polynomials P, $\mu(P)$ can be arbitrarily close to zero. For higher Mahler measures [LS11, Thm. 7] shows that for $k = 1, 2, \ldots$ the measure $\mu_{2k+1}\left((x^n-1)/(x-1)\right)$ does tend to zero as n goes to infinity.

It was shown in (6.10) that for positive integers k,

$$\pi\,\mu(1+x+y_1, 1+x+y_2, \ldots, 1+x+y_k) = \mathrm{Ls}_{k+1}\left(\frac{\pi}{3}\right) - \mathrm{Ls}_{k+1}\left(\pi\right). \tag{6.77}$$

This rapidly tends to zero with k since $|\,\mathrm{Ls}_{k+1}\left(\frac{\pi}{3}\right) - \mathrm{Ls}_{k+1}\left(\pi\right)| \leqslant \frac{2\pi}{3}\log^k 2$. Can one find any natural polynomial sequences so that $\mu(P_n, Q_n)$ tends to zero with n and so generalize [LS11, Thm. 7] ?

Chapter 7

Log-sine evaluations of Mahler measures, II

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[BBSW12] *Log-sine evaluations of Mahler measures, part II*
(with David Borwein, Jonathan M. Borwein, James Wan)
to appear in Integers (Selfridge memorial volume)

Abstract We continue our analysis of higher and multiple Mahler measures using log-sine integrals as started in [BS11a, BS11c]. This motivates a detailed study of various multiple polylogarithms [BBBL01] and worked examples are given. Our techniques enable the reduction of several multiple Mahler measures, and supply an easy proof of two conjectures by Boyd.

7.1 Introduction

In [BS11a] the classical log-sine integrals and their extensions were used to develop a variety of results relating to higher and multiple Mahler measures [Boy81, KLO08]. The utility of this approach was such that we continue the work herein. Among other things, it allows us to tap into a rich analytic literature [Lew81]. In [BS11c] the computational underpinnings of such studies are illuminated. The use of related integrals is currently being exploited for multi-zeta value studies [Ona11]. Such evaluations are also useful for physics [KS05]: log-sine integrals appeared for instance in the calculation of higher terms in the ε-expansion of various Feynman diagrams [Dav00, Kal05]. Of particular importance are the log-sine integrals at the special values $\pi/3$, $\pi/2$, $2\pi/3$, and π. The log-sine integrals also come up in many settings in number theory and analysis: classes of inverse binomial sums can be expressed in terms of generalized log-sine integrals [BBK01, DK04].

The structure of this article is as follows. In Section 7.2 our basic tools are described. After providing necessary results on log-sine integrals in Section 7.3, we turn to relationships between random walks and Mahler measures in Section 7.4. In particular, we will be interested in the multiple Mahler measure $\mu_n(1+x+y)$ which has a fine hypergeometric generating function (7.21) and a natural trigonometric representation (7.23) as a double integral.

In Section 7.5 we directly expand (7.21) and use known results from the ε-expansion of hypergeometric functions [DK01, DK04] to obtain $\mu_n(1 + x + y)$ in terms of multiple inverse binomial sums. In the cases $n = 1, 2, 3$ this leads to explicit polylogarithmic evaluations.

An alternative approach based of the double integral representation (7.23) is taken up in Section 7.6 which considers the evaluation of the inner integral in (7.23). Aided by combinatorics, we show in Theorems 7.6.3 and 7.6.12 that these can always be expressed in terms of multiple harmonic polylogarithms of weight k. Accordingly, we demonstrate in Section 7.6.3 how these polylogarithms can be reduced explicitly for low weights. In Section 7.7.1 we reprise from [BS11a] the evaluation of $\mu_2(1+x+y)$. Then in Section 7.7.2 we apply our general results from Section 7.6 to a conjectural evaluation of $\mu_3(1+x+y)$.

In Section 7.8 we finish with an elementary proof of two recently established 1998 conjectures of Boyd and use these tools to obtain a new Mahler measure.

7.2 Preliminaries

For k functions (typically Laurent polynomials) in n variables the *multiple Mahler measure*, introduced in [KLO08], is defined as

$$\mu(P_1, P_2, \ldots, P_k) := \int_0^1 \cdots \int_0^1 \prod_{j=1}^{k} \log \left| P_j \left(e^{2\pi i t_1}, \ldots, e^{2\pi i t_n} \right) \right| \mathrm{d}t_1 \mathrm{d}t_2 \ldots \mathrm{d}t_n.$$

When $P = P_1 = P_2 = \cdots = P_k$ this devolves to a *higher Mahler measure*, $\mu_k(P)$, as introduced and examined in [KLO08]. When $k = 1$ both reduce to the standard (logarithmic) *Mahler measure* [Boy81].

We also recall *Jensen's formula*:

$$\int_0^1 \log \left| \alpha - e^{2\pi i\, t} \right| \, \mathrm{d}t = \log \left(|\alpha| \vee 1 \right), \tag{7.1}$$

where $x \vee y = \max(x, y)$. An easy consequence of Jensen's formula is that for complex constants a and b we have

$$\mu(ax + b) = \log |a| \vee \log |b|. \tag{7.2}$$

7.3 Log-sine integrals

For $n = 1, 2, \ldots$, we consider the *log-sine integrals* defined by

$$\mathrm{Ls}_n \left(\sigma \right) := - \int_0^{\sigma} \log^{n-1} \left| 2 \sin \frac{\theta}{2} \right| \, \mathrm{d}\theta \tag{7.3}$$

and, for $k = 0, 1, \ldots, n-1$, their generalized versions

$$\mathrm{Ls}_n^{(k)} \left(\sigma \right) := - \int_0^{\sigma} \theta^k \, \log^{n-1-k} \left| 2 \sin \frac{\theta}{2} \right| \, \mathrm{d}\theta. \tag{7.4}$$

This is the notation used by Lewin [Lew58, Lew81]. In each case the modulus is not needed for $0 \leqslant \sigma \leqslant 2\pi$.

We observe that $\mathrm{Ls}_1(\sigma) = -\sigma$ and that $\mathrm{Ls}_n^{(0)}(\sigma) = \mathrm{Ls}_n(\sigma)$. In particular,

$$\mathrm{Ls}_2(\sigma) = \mathrm{Cl}_2(\sigma) := \sum_{n=1}^{\infty} \frac{\sin(n\sigma)}{n^2} \tag{7.5}$$

is the Clausen function introduced in (1.14). Various log-sine integral evaluations may be found in [Lew81, §7.6 & §7.9].

7.3.1 Log-sine integrals at π

We first recall that the log-sine integrals at π can always be evaluated in terms of zeta values. This is a consequence of the exponential generating function [Lew81, Eqn. (7.109)]

$$-\frac{1}{\pi} \sum_{m=0}^{\infty} \mathrm{Ls}_{m+1}(\pi) \frac{u^m}{m!} = \frac{\Gamma(1+u)}{\Gamma^2\left(1+\frac{u}{2}\right)} = \binom{u}{u/2}. \tag{7.6}$$

This will be revisited and put in context in Section 7.4. Here we only remark that, by the very definition, log-sine integrals at π correspond to very basic multiple Mahler measures:

$$\mu_m(1+x) = -\frac{1}{\pi} \mathrm{Ls}_{m+1}(\pi) \tag{7.7}$$

Example 7.3.1 (Values of $\mathrm{Ls}_n(\pi)$)**.** For instance, we have $\mathrm{Ls}_2(\pi) = 0$ as well as

$$\begin{aligned}
-\mathrm{Ls}_3(\pi) &= \frac{1}{12}\pi^3 \\
\mathrm{Ls}_4(\pi) &= \frac{3}{2}\pi\,\zeta(3) \\
-\mathrm{Ls}_5(\pi) &= \frac{19}{240}\pi^5 \\
\mathrm{Ls}_6(\pi) &= \frac{45}{2}\pi\,\zeta(5) + \frac{5}{4}\pi^3\zeta(3) \\
-\mathrm{Ls}_7(\pi) &= \frac{275}{1344}\pi^7 + \frac{45}{2}\pi\,\zeta^2(3) \\
\mathrm{Ls}_8(\pi) &= \frac{2835}{4}\pi\,\zeta(7) + \frac{315}{8}\pi^3\zeta(5) + \frac{133}{32}\pi^5\zeta(3),
\end{aligned}$$

and so forth. Note that these values may be conveniently obtained from (7.6) by a computer algebra system as the following snippet of *Maple* code demonstrates:

```
for k to 6 do simplify(subs(x=0,diff(Pi*binomial(x,x/2),x$k))) od;
```

More general log-sine evaluations with an emphasis on automatic evaluations have been studied in [BS11c]. ♢

For general log-sine integrals, the following computationally effective exponential generating function was obtained in [BS11c].

Theorem 7.3.2 (Generating function for $\mathrm{Ls}_{n+k+1}^{(k)}(\pi)$)**.** *For $2|\mu| < \lambda < 1$ we have*

$$\sum_{n,k\geqslant 0} \mathrm{Ls}_{n+k+1}^{(k)}(\pi)\,\frac{\lambda^n}{n!}\frac{(i\mu)^k}{k!} = -i\sum_{n\geqslant 0}\binom{\lambda}{n}\frac{(-1)^n\,\mathrm{e}^{i\pi\frac{\lambda}{2}} - \mathrm{e}^{i\pi\mu}}{\mu - \frac{\lambda}{2} + n}. \tag{7.8}$$

One may extract one-variable generating functions from (7.8). For instance,

$$\sum_{n=0}^{\infty} \mathrm{Ls}_{n+2}^{(1)}(\pi)\,\frac{\lambda^n}{n!} = \sum_{n=0}^{\infty}\binom{\lambda}{n}\frac{-1 + (-1)^n\cos\frac{\pi\lambda}{2}}{\left(n - \frac{\lambda}{2}\right)^2}.$$

The log-sine integrals at $\pi/3$ are especially useful as illustrated in [BBK01] and are discussed at some length in [BS11a] where other applications to Mahler measures are given.

7.3.2 Extensions of the log-sine integrals

It is possible to extend some of these considerations to the log-sine-cosine integrals

$$\mathrm{Lsc}_{m,n}(\sigma) := -\int_0^\sigma \log^{m-1}\left|2\,\sin\frac{\theta}{2}\right| \log^{n-1}\left|2\,\cos\frac{\theta}{2}\right| \mathrm{d}\theta. \tag{7.9}$$

Then $\mathrm{Lsc}_{m,1}(\sigma) = \mathrm{Ls}_m(\sigma)$ and $\mathrm{Lsc}_{m,n}(\sigma) = \mathrm{Lsc}_{n,m}(\sigma)$. As in (7.7), these are related to basic multiple Mahler measures. Namely, if we set

$$\mu_{m,n}(1-x, 1+x) := \mu(\underbrace{1-x, \cdots, 1-x}_{m}, \underbrace{1+x, \cdots, 1+x}_{n}) \tag{7.10}$$

then, immediately from the definition, we obtain the following:

Theorem 7.3.3 (Evaluation of $\mu_{m,n}(1-x,1+x)$)**.** *For non-negative integers m, n,*

$$\mu_{m,n}(1-x, 1+x) = -\frac{1}{\pi}\,\mathrm{Lsc}_{m+1,n+1}(\pi)\,. \tag{7.11}$$

In every case this is evaluable in terms of zeta values. Indeed, using the result in [Lew81, §7.9.2, (7.114)], we obtain the generating function

$$\mathrm{gs}(u,v) := -\frac{1}{\pi}\sum_{m,n=0}^{\infty} \mathrm{Lsc}_{m+1,n+1}(\pi)\,\frac{u^m}{m!}\frac{v^n}{n!} = \frac{2^{u+v}}{\pi}\,\frac{\Gamma\left(\frac{1+u}{2}\right)\Gamma\left(\frac{1+v}{2}\right)}{\Gamma\left(1+\frac{u+v}{2}\right)}. \tag{7.12}$$

From the duplication formula for the gamma function this can be rewritten as

$$\mathrm{gs}(u,v) = \binom{u}{u/2}\binom{v}{v/2}\frac{\Gamma\left(1+\frac{u}{2}\right)\Gamma\left(1+\frac{v}{2}\right)}{\Gamma\left(1+\frac{u+v}{2}\right)},$$

so that

$$\mathrm{gs}(u,0) = \binom{u}{u/2} = \mathrm{gs}(u,u).$$

From here it is apparent that (7.12) is an extension of (7.6):

Example 7.3.4 (Values of $\mathrm{Lsc}_{n,m}(\pi)$)**.** For instance,

$$\mu_{2,1}(1-x,1+x) = \mu_{1,2}(1-x,1+x) = \frac{1}{4}\zeta(3),$$
$$\mu_{3,2}(1-x,1+x) = \frac{3}{4}\zeta(5) - \frac{1}{8}\pi^2\zeta(3),$$
$$\mu_{6,3}(1-x,1+x) = \frac{315}{4}\zeta(9) + \frac{135}{32}\pi^2\zeta(7) + \frac{309}{128}\pi^4\zeta(5) - \frac{45}{256}\pi^6\zeta(3) - \frac{1575}{32}\zeta^3(3).$$

As in Example 7.3.1 this can be easily obtained with a line of code in a computer algebra system such as *Mathematica* or *Maple*. ♢

Remark 7.3.5. From $\mathrm{gs}(u,-u) = \sec(\pi u/2)$ we may deduce that, for $n = 0,1,2,\ldots$,

$$\sum_{k=0}^{n}(-1)^k\mu_{k,n-k}(1-x,1+x) = |E_{2n}|\,\frac{\left(\frac{\pi}{2}\right)^{2n}}{(2n)!} = \frac{4}{\pi}\,L_{-4}(2n+1),$$

where E_{2n} are the even Euler numbers: $1,-1,5,-61,1385\ldots.$ ♢

A more recondite *extended log-sine integral of order three* is developed in [Lew81, §8.4.3] from properties of the trilogarithm. It is defined by

$$\mathrm{Ls}_3(\theta,\omega) := -\int_0^\theta \log\left|2\sin\frac{\sigma}{2}\right|\,\log\left|2\sin\frac{\sigma+\omega}{2}\right|\,\mathrm{d}\sigma, \tag{7.13}$$

so that $\mathrm{Ls}_3(\theta, 0) = \mathrm{Ls}_3(\theta)$. This extended log-sine integral reduces as follows:

$$\begin{aligned} -\mathrm{Ls}_3(2\theta, 2\omega) = {} & \frac{1}{2}\mathrm{Ls}_3(2\omega) - \frac{1}{2}\mathrm{Ls}_3(2\theta) - \frac{1}{2}\mathrm{Ls}_3(2\theta + 2\omega) \\ & - 2\,\mathrm{Im}\,\mathrm{Li}_3\left(\frac{\sin(\theta)\mathrm{e}^{i\omega}}{\sin(\theta+\omega)}\right) + \theta\log^2\left(\frac{\sin(\theta)}{\sin(\theta+\omega)}\right) \\ & + \log\left(\frac{\sin(\theta)}{\sin(\theta+\omega)}\right)\{\mathrm{Cl}_2(2\theta) + \mathrm{Cl}_2(2\omega) - \mathrm{Cl}_2(2\theta+2\omega)\}. \end{aligned} \tag{7.14}$$

We note that $-\frac{1}{2\pi}\mathrm{Ls}_3(2\pi, \omega) = \mu(1-x, 1-e^{i\omega}x)$ but this is more easily evaluated by Fourier techniques. Indeed one has:

Proposition 7.3.6 (A dilogarithmic measure, part I [KLO08])**.** *For two complex numbers u and v we have*

$$\mu(1-u\,x, 1-v\,x) = \begin{cases} \frac{1}{2}\,\mathrm{Re}\,\mathrm{Li}_2(v\overline{u}), & \textit{if } |u| \leqslant 1, |v| \leqslant 1, \\ \frac{1}{2}\,\mathrm{Re}\,\mathrm{Li}_2\left(\frac{v}{u}\right), & \textit{if } |u| \geqslant 1, |v| \leqslant 1, \\ \frac{1}{2}\,\mathrm{Re}\,\mathrm{Li}_2\left(\frac{1}{v\overline{u}}\right) + \log|u|\log|v|, & \textit{if } |u| \geqslant 1, |v| \geqslant 1. \end{cases} \tag{7.15}$$

This is proven much as is (7.75) of Proposition 7.7.2. In Lewin's terms [Lew81, A.2.5] for $0 < \theta \leqslant 2\pi$ and $r \geqslant 0$ we may write

$$\mathrm{Re}\,\mathrm{Li}_2\left(re^{i\theta}\right) =: \mathrm{Li}_2(r, \theta) = -\frac{1}{2}\int_0^r \log\left(t^2 + 1 - 2t\cos\theta\right)\frac{\mathrm{d}t}{t}, \tag{7.16}$$

with the reflection formula

$$\mathrm{Li}_2(r, \theta) + \mathrm{Li}_2\left(\frac{1}{r}, \theta\right) = \zeta(2) - \frac{1}{2}\log^2 r + \frac{1}{2}(\pi - \theta)^2. \tag{7.17}$$

This leads to:

Proposition 7.3.7 (A dilogarithmic measure, part II)**.** *For complex numbers $u = re^{i\theta}$*

and $v = se^{i\tau}$ *we have*

$$\mu(1-u\,x, 1-v\,x) = \begin{cases} \frac{1}{2}\operatorname{Li}_2\left(rs, \theta-\tau\right) & \textit{if } r \leqslant 1, s \leqslant 1, \\ \frac{1}{2}\operatorname{Li}_2\left(\frac{s}{r}, \theta+\tau\right), & \textit{if } r \geqslant 1, s \leqslant 1, \\ \frac{1}{2}\operatorname{Li}_2\left(\frac{1}{sr}, \theta-\tau\right) + \log r \log s, & \textit{if } r \geqslant 1, s \geqslant 1. \end{cases} \tag{7.18}$$

We remark that Proposition 7.3.7 and equation (7.17) allow for efficient numerical computation.

7.4 Mahler measures and moments of random walks

The s-th moments of an n-step uniform random walk are given by

$$W_n(s) = \int_0^1 \cdots \int_0^1 \left|\sum_{k=1}^n e^{2\pi i t_k}\right|^s \mathrm{d}t_1 \cdots \mathrm{d}t_n$$

and their relation with Mahler measure is observed in [BSWZ11]. In particular,

$$W_n'(0) = \mu(1 + x_1 + \ldots + x_{n-1}),$$

with the cases $2 \leqslant n \leqslant 6$ discussed in [BS11a].

Higher derivatives of W_n correspond to higher Mahler measures:

$$W_n^{(m)}(0) = \mu_m(1 + x_1 + \ldots + x_{n-1}). \tag{7.19}$$

The evaluation $W_2(s) = \binom{s}{s/2}$ thus explains and proves the generating function (7.6); in other words, we find that

$$W_2^{(m)}(0) = -\frac{1}{\pi}\,\mathrm{Ls}_{m+1}(\pi)\,. \tag{7.20}$$

As a consequence of the study of random walks in [BSWZ11] we record the following generating function for $\mu_m(1+x+y)$ which follows from (7.19) and the hypergeometric expression for W_3 in [BSWZ11]. There is a corresponding expression for W_4, the generating function of $\mu_m(1+x+y+z)$, in terms of a single Meijer-G function [BSWZ11].

Theorem 7.4.1 (Hypergeometric form for $W_3(s)$)**.** *For complex $|s| < 2$, we may write*

$$W_3(s) = \sum_{n=0}^{\infty} \mu_n(1+x+y)\frac{s^n}{n!} = \frac{\sqrt{3}}{2\pi}\,3^{s+1}\,\frac{\Gamma(1+\frac{s}{2})^2}{\Gamma(s+2)}\,{}_3F_2\left(\left.{\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2} \atop 1, \frac{s+3}{2}}\right|\frac{1}{4}\right) \tag{7.21}$$

$$= \frac{\sqrt{3}}{\pi}\left(\frac{3}{2}\right)^{s+1}\int_0^1 \frac{z^{1+s}\,{}_2F_1\left(\left.{1+\frac{s}{2}, 1+\frac{s}{2} \atop 1}\right|\frac{z^2}{4}\right)}{\sqrt{1-z^2}}\,\mathrm{d}z. \tag{7.22}$$

Proof. Equation (7.21) is proven in [BSWZ11], while (7.22) is a consequence of (7.21) and [OLBC10, Eqn. (16.5.2)]. □

We shall exploit Theorem 7.4.1 next, in Section 7.5. For integers $n \geqslant 1$ we also have

$$\mu_n(1+x+y) = \frac{1}{4\pi^2}\int_0^{2\pi}\mathrm{d}\theta\int_0^{2\pi}\left(\mathrm{Re}\,\log\left(1-2\sin(\theta)\mathrm{e}^{i\,\omega}\right)\right)^n\,\mathrm{d}\omega, \tag{7.23}$$

as follows directly from the definition and some simple trigonometry, since $\mathrm{Re}\,\log z = \log|z|$. This is the basis for the evaluations of Section 7.6. In particular, in Section 7.6 we will evaluate the inner integral in terms of multiple harmonic polylogarithms.

7.5 Epsilon expansion of W_3

In this section we use known results from the ε-expansion of hypergeometric functions [DK01, DK04] to obtain $\mu_n(1+x+y)$ in terms of multiple inverse binomial sums. We then derive complete evaluations of $\mu_1(1+x+y)$, $\mu_2(1+x+y)$ and $\mu_3(1+x+y)$. An alternative approach will be pursued in Sections 7.6 and 7.7.

In light of Theorem 7.4.1, the evaluation of $\mu_n(1+x+y)$ is essentially reduced to the Taylor expansion

$$ {}_3F_2\left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4} \right) = \sum_{n=0}^{\infty} \alpha_n \varepsilon^n. \tag{7.24} $$

Indeed, from (7.21) and Leibniz' rule we have

$$ \mu_n(1+x+y) = \frac{\sqrt{3}}{2\pi} \sum_{k=0}^{n} \binom{n}{k} \alpha_k \beta_{n-k} \tag{7.25} $$

where β_k is defined by

$$ 3^{\varepsilon+1} \frac{\Gamma(1+\frac{\varepsilon}{2})^2}{\Gamma(2+\varepsilon)} = \sum_{n=0}^{\infty} \beta_n \varepsilon^n. \tag{7.26} $$

Note that β_k is easy to compute as illustrated in Example 7.3.1. The expansion of hypergeometric functions in terms of their parameters as in (7.24) occurs in physics [DK01, DK04] in the context of the evaluation of Feynman diagrams and is commonly referred to as *epsilon expansion*, thus explaining the choice of variable in (7.24).

Remark 7.5.1. From (7.26) we see that the β_n may be computed directly from the coefficients γ_n defined by the Taylor expansion

$$ \frac{\Gamma(1+\frac{\varepsilon}{2})^2}{\Gamma(1+\varepsilon)} = \frac{1}{\binom{\varepsilon}{\varepsilon/2}} = \sum_{n=0}^{\infty} \gamma_n \varepsilon^n. $$

Appealing to (7.6) we find that γ_n is recursively determined by $\gamma_0 = 1$ and

$$\gamma_n = \frac{1}{\pi} \sum_{k=1}^{n} \mathrm{Ls}_{k+1}(\pi) \frac{\gamma_{n-k}}{k!}.$$

In particular, the results of Section 7.3.1 show that γ_n can always be expressed in terms of zeta values. Accordingly, β_n evaluates in terms of $\log 3$ and zeta values. $\Diamond$

Let $S_k(j) := \sum_{m=1}^{j} \frac{1}{m^k}$ denote the harmonic numbers of order k. Following [DK04] we abbreviate $S_k := S_k(j-1)$ and $\bar{S}_k := S_k(2j-1)$ in order to make it more clear which results in this reference contribute to the evaluations below. As in [DK01, Appendix B], we use the duplication formula $(2a)_{2j} = 4^j (a)_j (a+1/2)_j$ as well as the expansion

$$\frac{(m+a\varepsilon)_j}{(m)_j} = \exp\left[-\sum_{k=1}^{\infty} \frac{(-a\varepsilon)^k}{k} \left[S_k(j+m-1) - S_k(m-1)\right]\right], \tag{7.27}$$

for m a positive integer, to write

$$\begin{aligned}
{}_3F_2\left(\begin{matrix}\frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2}\end{matrix}\middle|\frac{1}{4}\right) &= \sum_{j=0}^{\infty} \frac{(1+\varepsilon/2)_j^3}{4^j (j!)^2 (3/2+\varepsilon/2)_j} \\
&= \sum_{j=0}^{\infty} \frac{(1+\varepsilon/2)_j^4}{(j!)^2 (2+\varepsilon)_{2j}} \\
&= \sum_{j=0}^{\infty} \frac{2}{j+1} \frac{1}{\binom{2(j+1)}{j+1}} \left[\frac{(1+\varepsilon/2)_j}{j!}\right]^4 \left[\frac{(2+\varepsilon)_{2j}}{(2j+1)!}\right]^{-1} \\
&= \sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} \exp\left[\sum_{k=1}^{\infty} \frac{(-\varepsilon)^k}{k} A_{k,j}\right]
\end{aligned} \tag{7.28}$$

where

$$A_{k,j} := S_k(2j-1) - 1 - 4\frac{S_k(j-1)}{2^k} = \sum_{m=2}^{2j-1} \frac{2(-1)^{m+1} - 1}{m^k}. \tag{7.29}$$

We can now read off the terms α_n of the ε-expansion (7.24):

Theorem 7.5.2. *For $n = 0, 1, 2, \ldots$*

$$\alpha_n = [\varepsilon^n]\, {}_3F_2 \left(\left. \begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \right| \frac{1}{4} \right) = (-1)^n \sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} \sum \prod_{k=1}^{n} \frac{A_{k,j}^{m_k}}{m_k! k^{m_k}} \tag{7.30}$$

where the inner sum is over all non-negative integers $m_1, \ldots, m_n$ such that $m_1 + 2m_2 + \ldots + nm_n = n$.

Proof. Equation (7.30) may be derived from (7.28) using, for instance, Faà di Bruno's formula for the n-th derivative of the composition of two functions. □

Example 7.5.3 (α_0, α_1 and α_2)**.** In particular,

$$\begin{aligned} \alpha_1 = [\varepsilon]\, {}_3F_2 \left(\left. \begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \right| \frac{1}{4} \right) &= -\sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} A_{1,j} \\ &= -\sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} \left[\bar{S}_1 - 2S_1 - 1 \right]. \end{aligned}$$

Such *multiple inverse binomial sums* are studied in [DK04]. In particular, using [DK04, (2.20), (2.21)] we find

$$\alpha_0 = \frac{2\pi}{3\sqrt{3}}, \tag{7.31}$$

$$\alpha_1 = \frac{2}{3\sqrt{3}} \left[\pi - \pi \log 3 + \mathrm{Ls}_2 \left(\frac{\pi}{3} \right) \right]. \tag{7.32}$$

For the second term α_2 in the ε-expansion (7.28) produces

$$\begin{aligned} [\varepsilon^2]\, {}_3F_2 \left(\left. \begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \right| \frac{1}{4} \right) &= \sum_{j=1}^{\infty} \frac{1}{j} \frac{1}{\binom{2j}{j}} \left[A_{1,j}^2 + A_{2,j} \right] \\ &= \sum_{j=1}^{\infty} \frac{1}{j} \frac{1}{\binom{2j}{j}} \left[\bar{S}_2 - S_2 + (\bar{S}_1 - 2S_1)^2 - 2\bar{S}_1 + 4S_1 \right]. \end{aligned}$$

Using [DK04, (2.8),(2.22)–(2.24)] we obtain

$$\alpha_2 = \frac{2}{3\sqrt{3}}\left[\frac{\pi}{72} - \pi\log 3 + \frac{1}{2}\pi\log 3 + (1-\log 3)\,\mathrm{Ls}_2\left(\frac{\pi}{3}\right)\right.$$
$$\left. + \frac{3}{2}\,\mathrm{Ls}_3\left(\frac{\pi}{3}\right) + \frac{3}{2}\,\mathrm{Ls}_3\left(\frac{2\pi}{3}\right) - 3\,\mathrm{Ls}_3\left(\pi\right)\right]. \tag{7.33}$$

$\diamondsuit$

These results provide us with evaluations of $\mu_1(1+x+y)$ and $\mu_2(1+x+y)$ as given next. As expected, the result for $\mu_1(1+x+y)$ agrees with Smyth's original evaluation, and the result for $\mu_2(1+x+y)$ agrees with our prior evaluation in [BS11a]. The latter evaluation will be recalled in Section 7.7.1.

Theorem 7.5.4 (Evaluation of $\mu_1(1+x+y)$ and $\mu_2(1+x+y)$)**.** *We have*

$$\mu_1(1+x+y) = \frac{1}{\pi}\,\mathrm{Ls}_2\left(\frac{\pi}{3}\right), \tag{7.34}$$
$$\mu_2(1+x+y) = \frac{3}{\pi}\,\mathrm{Ls}_3\left(\frac{2\pi}{3}\right) + \frac{\pi^2}{4}. \tag{7.35}$$

Proof. Using Theorem 7.4.1 we obtain

$$\mu_1(1+x+y) = \frac{3\sqrt{3}}{2\pi}\left[(\log 3 - 1)\alpha_0 + \alpha_1\right]. \tag{7.36}$$

Combining this with equations (7.31) and (7.32) yields (7.34).

Again using Theorem 7.4.1 we find

$$\mu_2(1+x+y) = \frac{3\sqrt{3}}{2\pi}\left[(\log^2 3 - 2\log 3 + 2 - \tfrac{\pi^2}{12})\alpha_0 + 2(\log 3 - 1)\alpha_1 + 2\alpha_2\right] \tag{7.37}$$

and, together with equations (7.31), (7.32) and (7.33), arrive at

$$\begin{aligned}\pi\mu_2(1+x+y) &= 3\,\mathrm{Ls}_3\left(\frac{2\pi}{3}\right)+3\,\mathrm{Ls}_3\left(\frac{\pi}{3}\right)-6\,\mathrm{Ls}_3\left(\pi\right)-\frac{\pi^3}{18}\\ &= 3\,\mathrm{Ls}_3\left(\frac{2\pi}{3}\right)+\frac{\pi^3}{4}.\end{aligned}\tag{7.38}$$

The last equality follows, for instance, automatically from the results in [BS11c]. □

Example 7.5.5 (α_3)**.** The evaluation of α_3 is more involved and we omit some details. Again, (7.28) produces

$$[\varepsilon^3]\ {}_3F_2\left(\begin{matrix}\frac{\varepsilon+2}{2},\frac{\varepsilon+2}{2},\frac{\varepsilon+2}{2}\\ 1,\frac{\varepsilon+3}{2}\end{matrix}\middle|\frac{1}{4}\right)=-\frac{1}{3}\sum_{j=1}^{\infty}\frac{1}{j}\frac{1}{\binom{2j}{j}}\left[A_{1,j}^3+3A_{1,j}A_{2,j}+2A_{3,j}\right].$$

Using [DK04, (2.25)–(2.28),(2.68)–(2.70),(2.81),(2.89)] as well as results from [BS11c] we are lead to

$$\begin{aligned}\alpha_3=\frac{2}{3\sqrt{3}}\Bigg[&\frac{5\pi^3}{108}(1-\log 3)+\frac{1}{2}\pi\log^2 3-\frac{1}{6}\pi\log^3 3+\frac{11}{9}\pi\zeta(3)\\ &+\mathrm{Cl}_2\left(\frac{\pi}{3}\right)\left(\frac{5}{36}\pi^2-\log 3+\frac{1}{2}\log^2 3\right)-3\,\mathrm{Gl}_{2,1}\left(\frac{2\pi}{3}\right)(1-\log 3)\\ &-\frac{35}{6}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right)+15\,\mathrm{Cl}_{2,1,1}\left(\frac{2\pi}{3}\right)-3\,\mathrm{Lsc}_{2,3}\left(\frac{\pi}{3}\right)\Bigg].\end{aligned}\tag{7.39}$$

Observe the occurrence of the log-sine-cosine integral $\mathrm{Lsc}_{2,3}\left(\frac{\pi}{3}\right)$. These integrals were defined in (7.9). ◊

Proceeding as in the proof of Theorem 7.5.4 we obtain:

Theorem 7.5.6 (Evaluation of $\mu_3(1+x+y)$)**.** *We have*

$$\begin{aligned}\pi\mu_3(1+x+y) &= 15\,\mathrm{Ls}_4\left(\frac{2\pi}{3}\right)-18\,\mathrm{Lsc}_{2,3}\left(\frac{\pi}{3}\right)-15\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right)\\ &\quad-\frac{1}{4}\pi^2\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)-17\pi\zeta(3).\end{aligned}\tag{7.40}$$

The log-sine-cosine integral $\mathrm{Lsc}_{2,3}\left(\frac{\pi}{3}\right)$ appears to reduce further as

$$12\,\mathrm{Lsc}_{2,3}\left(\frac{\pi}{3}\right) \overset{?[1]}{=} 6\,\mathrm{Ls}_4\left(\frac{2\pi}{3}\right) - 4\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right) - 7\pi\zeta(3) \tag{7.41}$$
$$= 6\,\mathrm{Ls}_4\left(\frac{2\pi}{3}\right) - \frac{8}{9}\,\mathrm{Ls}_4\left(\frac{\pi}{3}\right) - \frac{59}{9}\pi\zeta(3).$$

This conjectural reduction also appears in [DK01, (A.30)] where it was found via PSLQ. Combining this with (7.40), we obtain an conjectural evaluation of $\mu_3(1+x+y)$ equivalent to (7.81).

On the other hand, it follows from [DK04, (2.18)] that

$$12\,\mathrm{Lsc}_{2,3}\left(\frac{\pi}{3}\right) = \mathrm{Ls}_4\left(\frac{2\pi}{3}\right) - 4\,\mathrm{Ls}_4\left(\frac{\pi}{3}\right) - \frac{1}{12}\pi\log^3 3$$
$$+ 24\,\mathrm{Ti}\,4\frac{1}{\sqrt{3}} + 12\log 3\,\mathrm{Ti}\,3\frac{1}{\sqrt{3}} + 3\log^2 3\,\mathrm{Ti}\,2\frac{1}{\sqrt{3}}. \tag{7.42}$$

Using the known evaluations — see for instance [BS11a, (76),(77)] — for the inverse tangent integrals of order two and three, we find that (7.41) is equivalent to

$$\mathrm{Ti}\,4\frac{1}{\sqrt{3}} \overset{?[1]}{=} \frac{5}{24}\,\mathrm{Ls}_4\left(\frac{2\pi}{3}\right) + \frac{7}{54}\,\mathrm{Ls}_4\left(\frac{\pi}{3}\right) - \frac{59}{216}\pi\zeta(3) - \frac{1}{288}\pi\log^3 3$$
$$- \frac{1}{2}\log 3\,\mathrm{Ti}\,3\frac{1}{\sqrt{3}} - \frac{1}{8}\log^2 3\,\mathrm{Ti}\,2\frac{1}{\sqrt{3}}. \tag{7.43}$$

7.6 Trigonometric analysis of $\mu_n(1+x+y)$

As promised in [BS11a] — motivated by the development outlined above — we take the analysis of $\mu_n(1+x+y)$ for $n \geqslant 3$ a fair distance. In light of (7.23) we define

$$\rho_n(\alpha) := \frac{1}{2\pi}\int_{-\pi}^{\pi} \left(\mathrm{Re}\,\log\left(1-\alpha\,\mathrm{e}^{i\omega}\right)\right)^n\,\mathrm{d}\omega \tag{7.44}$$

for $n \geqslant 0$ so that

$$\mu_n(1+x+y) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \rho_n(|2\sin\theta|)\,\mathrm{d}\theta. \tag{7.45}$$

We thus typically set $\alpha = |2\sin\theta|$. Note that $\rho_0(\alpha) = 1$, $\rho_1(\alpha) = \log(|\alpha| \vee 1)$.

Proposition 7.6.1 (Properties of ρ_n)**.** *Let n be a positive integer.*

(a) For $|\alpha| \leqslant 1$ we have

$$\rho_n(\alpha) = (-1)^n \sum_{m=1}^{\infty} \frac{\alpha^m}{m^n}\,\omega_n(m), \tag{7.46}$$

where ω_n is defined as

$$\omega_n(m) = \sum_{\sum_{j=1}^n k_j = m} \frac{1}{2\pi}\int_{-\pi}^{\pi} \prod_{j=1}^{n} \frac{m}{k_j}\cos(k_j\omega)\,\mathrm{d}\omega. \tag{7.47}$$

(b) For $|\alpha| \geqslant 1$ we have

$$\rho_n(\alpha) = \sum_{k=0}^{n} \binom{n}{k} \log^{n-k}|\alpha|\,\rho_k\left(\frac{1}{\alpha}\right). \tag{7.48}$$

Proof. For (a) we use (7.44) to write

$$\begin{aligned}
\rho_n(\alpha) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \left(\mathrm{Re}\ \log\left(1-\alpha \mathrm{e}^{i\,\omega}\right)\right)^n\,\mathrm{d}\omega \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} \left\{-\sum_{k\geqslant 1}\frac{\alpha^k}{k}\,\cos(k\omega)\right\}^n\,\mathrm{d}\omega \\
&= (-1)^n \sum_{m=1}^{\infty} \frac{\alpha^m}{m^n}\,\omega_n(m),
\end{aligned}$$

as asserted. We note that $|\omega_n(m)| \leqslant m^n$ and so the sum is convergent.

For (b) we now use (7.44) to write

$$\begin{aligned}
\rho_n(\alpha) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \log^n\left(|\alpha|\,\left|1-\alpha^{-1}\mathrm{e}^{i\,\omega}\right|\right)\,\mathrm{d}\omega \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} \left(\log|\alpha| + \log\left|1-\alpha^{-1}\mathrm{e}^{i\,\omega}\right|\right)^n\,\mathrm{d}\omega \\
&= \sum_{k=0}^{n}\binom{n}{k}\log^{n-k}|\alpha|\,\frac{1}{2\pi}\int_{-\pi}^{\pi}\log^k\left|1-\alpha^{-1}\mathrm{e}^{i\,\omega}\right|\,\mathrm{d}\omega \\
&= \sum_{k=0}^{n}\binom{n}{k}\log^{n-k}|\alpha|\,\rho_k\left(\frac{1}{\alpha}\right),
\end{aligned}$$

as required. ☐

Example 7.6.2 (Evaluation of ω_n and ρ_n for $n \leqslant 2$)**.** We have $\omega_0(m) = 0$, $\omega_1(m) = \delta_0(m)$, and

$$\omega_2(0) = 1, \quad \omega_2(2m) = 2, \quad \omega_2(2m+1) = 0. \tag{7.49}$$

Likewise, $\rho_0(\alpha) = 1$, $\rho_1(\alpha) = \log(|\alpha| \vee 1)$, and

$$\rho_2(\alpha) = \begin{cases} \frac{1}{2}\,\mathrm{Li}_2(\alpha^2) & \text{for } |\alpha| \leqslant 1, \\ \frac{1}{2}\,\mathrm{Li}_2\left(\frac{1}{\alpha^2}\right) + \log^2|\alpha| & \text{for } |\alpha| \geqslant 1, \end{cases} \tag{7.50}$$

where the latter follows from (7.49) and Proposition 7.6.1. ◊

We have arrived at the following description of $\mu_n(1+x+y)$:

Theorem 7.6.3 (Evaluation of $\mu_n(1+x+y)$)**.** *Let n be a positive integer. Then*

$$\begin{aligned}
\mu_n(1+x+y) = \frac{1}{\pi}\left\{\mathrm{Ls}_{n+1}\left(\frac{\pi}{3}\right) - \mathrm{Ls}_{n+1}(\pi)\right\} + \frac{2}{\pi}\int_0^{\pi/6}\rho_n(2\sin\theta)\,\mathrm{d}\theta \\
+ \frac{2}{\pi}\sum_{k=2}^{n}\binom{n}{k}\int_{\pi/6}^{\pi/2}\log^{n-k}(2\sin\theta)\,\rho_k\left(\frac{1}{2\sin\theta}\right)\mathrm{d}\theta.
\end{aligned} \tag{7.51}$$

Proof. Since $|\alpha| < 1$ exactly when $|\theta| < \pi/6$ we start with (7.45) to get

$$\begin{aligned}
\mu_n(1+x+y) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \rho_n(|2\sin\theta|)\,\mathrm{d}\theta \\
&= \frac{2}{\pi}\int_0^{\pi/6} \rho_n(2\sin\theta)\,\mathrm{d}\theta + \frac{2}{\pi}\int_{\pi/6}^{\pi/2} \rho_n(2\sin\theta)\,\mathrm{d}\theta \\
&= \frac{2}{\pi}\int_0^{\pi/6} \rho_n(2\sin\theta)\,\mathrm{d}\theta \\
&\quad + \sum_{k=0}^{n}\binom{n}{k}\frac{2}{\pi}\int_{\pi/6}^{\pi/2} \log^{n-k}(2\sin\theta)\,\rho_k\left(\frac{1}{2\sin\theta}\right)\,\mathrm{d}\theta.
\end{aligned}$$

We observe that for $k=1$ the contribution is zero since ρ_1 is zero for $|\alpha| < 1$. After evaluating the term with $k=0$ we arrive at (7.51). □

As is shown in [BS11a],

$$\frac{1}{\pi}\left\{\mathrm{Ls}_{n+1}\left(\frac{\pi}{3}\right) - \mathrm{Ls}_{n+1}(\pi)\right\} = \mu(1+x+y_1, 1+x+y_2, \ldots, 1+x+y_n)$$

is a multiple Mahler measure. While log-sine integrals at π were the subject of Example 7.3.1 we record the following for values at $\pi/3$:

Example 7.6.4 (Values of $\mathrm{Ls}_n(\pi/3)$)**.** The following evaluations may be obtained with the help of the implementation[1] accompanying [BS11c].

$$
\begin{aligned}
\mathrm{Ls}_2\left(\frac{\pi}{3}\right) &= \mathrm{Cl}_2\left(\frac{\pi}{3}\right)\\
-\mathrm{Ls}_3\left(\frac{\pi}{3}\right) &= \frac{7}{108}\,\pi^3\\
\mathrm{Ls}_4\left(\frac{\pi}{3}\right) &= \frac{1}{2}\pi\,\zeta(3) + \frac{9}{2}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right)\\
-\mathrm{Ls}_5\left(\frac{\pi}{3}\right) &= \frac{1543}{19440}\pi^5 - 6\,\mathrm{Gl}_{4,1}\left(\frac{\pi}{3}\right)\\
\mathrm{Ls}_6\left(\frac{\pi}{3}\right) &= \frac{15}{2}\pi\,\zeta(5) + \frac{35}{36}\,\pi^3\zeta(3) + \frac{135}{2}\,\mathrm{Cl}_6\left(\frac{\pi}{3}\right)\\
-\mathrm{Ls}_7\left(\frac{\pi}{3}\right) &= \frac{74369}{326592}\pi^7 + \frac{15}{2}\,\pi\zeta(3)^2 - 135\,\mathrm{Gl}_{6,1}\left(\frac{\pi}{3}\right)\\
\mathrm{Ls}_8\left(\frac{\pi}{3}\right) &= \frac{13181}{2592}\pi^5\zeta(3) + \frac{1225}{24}\pi^3\zeta(5) + \frac{319445}{864}\pi\zeta(7)\\
&\quad + \frac{35}{2}\pi^2\,\mathrm{Cl}_6\left(\frac{\pi}{3}\right) + \frac{945}{4}\,\mathrm{Cl}_8\left(\frac{\pi}{3}\right) + 315\,\mathrm{Cl}_{6,1,1}\left(\frac{\pi}{3}\right)
\end{aligned}
$$

$\lozenge$

7.6.1 Further evaluation of ρ_n

To make further progress, we need first to determine ρ_n for $n \geqslant 3$. It is instructive to explore the next few cases.

Example 7.6.5 (Evaluation of ω_3 and ρ_3)**.** We use

$$4\,\cos(a)\cos(b)\cos(c) = \cos(a+b+c) + \cos(a-b-c) + \cos(a-b+c) + \cos(a-c+b)$$

and so derive

$$\omega_3(m) = \frac{1}{4}\sum\left\{\frac{m^3}{ijk} : i \pm j \pm k = 0, i+j+k = m\right\}.$$

[1] Packages are available for download from http://arminstraub.com/pub/log-sine-integrals

Note that we must have exactly one of $i = j + k, j = k + i$ or $k = i + j$. We thus learn that $\omega_3(2m+1) = 0$. Moreover, by symmetry,

$$\begin{aligned}\omega_3(2m) &= \frac{3}{4}\sum_{j+k=m}\frac{(2m)^3}{jk(j+k)}\\ &= 6\sum_{j+k=m}\frac{m^2}{jk} = 12\,m\sum_{k=1}^{m-1}\frac{1}{k}.\end{aligned} \tag{7.52}$$

Hence, by Proposition 7.6.1,

$$\rho_3(\alpha) = -\frac{3}{2}\sum_{m=1}^{\infty}\frac{\sum_{k=1}^{m-1}\frac{1}{k}}{m^2}\,\alpha^{2m} = -\frac{3}{2}\,\mathrm{Li}_{2,1}(\alpha^2) \tag{7.53}$$

for $|\alpha| < 1$. ◊

7.6.2 A general formula for ρ_n

In the general case we have

$$\prod_{j=1}^{n}\cos(x_j) = 2^{-n}\sum_{\varepsilon\in\{-1,1\}^n}\cos\left(\sum_{j=1}^{n}\varepsilon_j x_j\right) \tag{7.54}$$

which follows inductively from $2\cos(a)\cos(b) = \cos(a+b) + \cos(a-b)$.

Proposition 7.6.6. *For integers $n, m \geqslant 0$ we have $\omega_n(2m+1) = 0$.*

Proof. In light of (7.54) the summand corresponding to the indices $k_1, \ldots, k_n$ in (7.47) for $\omega_n(2m+1) = 0$ is nonzero if and only if there exists $\varepsilon \in \{-1,1\}^n$ such that $\varepsilon_1 k_1 + \ldots + \varepsilon_n k_n = 0$. In other words, there is a set $S \subset \{1, \ldots, n\}$ such that

$$\sum_{j\in S} k_j = \sum_{j\notin S} k_j.$$

Thus $k_1 + \ldots + k_n = 2\sum_{j\in S} k_j$ which contradicts $k_1 + \ldots + k_n = 2m+1$. □

Example 7.6.7 (Evaluation of ω_4 and ρ_4)**.** Proceeding as in Example 7.6.5 and employing (7.54), we find

$$\begin{aligned}
\omega_4(2m) &= \frac{3}{8} \sum_{\substack{i+j=m \\ k+\ell=m}} \frac{(2m)^4}{ijk\ell} + \frac{1}{2} \sum_{i+j+k=m} \frac{(2m)^4}{ijk\ell} \\
&= 24m^2 \sum_{\substack{i<m \\ j<m}} \frac{1}{ij} + 24m^2 \sum_{i+j<m} \frac{1}{ij} \\
&= 48m^2 \sum_{i=1}^{m-1} \frac{1}{i} \sum_{j=1}^{i-1} \frac{1}{j} + 24m^2 \sum_{i=1}^{m-1} \frac{1}{i^2} + 48m^2 \sum_{i=1}^{m-1} \frac{1}{i} \sum_{j=1}^{i-1} \frac{1}{j}.
\end{aligned} \tag{7.55}$$

Consequently, for $|\alpha| < 1$ and appealing to Proposition 7.6.1,

$$\rho_4(\alpha) = \sum_{m=1}^{\infty} \frac{\alpha^{2m}}{(2m)^4} \omega_4(2m) = 6 \operatorname{Li}_{2,1,1}(\alpha^2) + \frac{3}{2} \operatorname{Li}_{2,2}(\alpha^2). \tag{7.56}$$

This suggests that $\rho_n(\alpha)$ is generally expressible as a sum of polylogarithmic terms, as will be shown next. $\Diamond$

To help the general evaluation of $\omega_n(2m)$, for integers $j \geqslant 0$ and $m \geqslant 1$, let us define

$$\sigma_j(m) := \sum_{m_1+\ldots+m_j=m} \frac{1}{m_1 \cdots m_j}. \tag{7.57}$$

Proposition 7.6.8. *For positive integers n, m we have*

$$\frac{\omega_n(2m)}{m^n} = \sum_{j=1}^{n-1} \binom{n}{j} \sigma_j(m) \sigma_{n-j}(m) \tag{7.58}$$

where σ_j is as defined in (7.57).

Proof. It follows from (7.54) that

$$\omega_n(2m) = \sum_{k_1+\ldots+k_n=2m} \sum_{\substack{\varepsilon \in \{-1,1\}^n \\ \sum_j \varepsilon_j k_j = 0}} \prod_{j=1}^{n} \frac{m}{k_j}.$$

Arguing as in Proposition 7.6.6 we therefore find that

$$\omega_n(2m) = \sum_{j=1}^{n-1} \binom{n}{j} \sum_{\substack{k_1+\ldots+k_j=m \\ k_{j+1}+\ldots+k_n=m}} \prod_{j=1}^{n} \frac{m}{k_j}.$$

This is equivalent to (7.58). □

Moreover, we have a simple useful recursion:

Proposition 7.6.9. *Let $m \geqslant 1$. Then $\sigma_1(m) = 1/m$ while for $j \geqslant 2$ we have*

$$\sigma_j(m) = \frac{j}{m} \sum_{r=1}^{m-1} \sigma_{j-1}(r).$$

Proof. We have

$$\begin{aligned}
\sigma_j(m) &= \sum_{m_1+\ldots+m_j=m} \frac{1}{m_1 \cdots m_j} \\
&= \frac{j}{m} \sum_{m_1+\ldots+m_j=m} \frac{1}{m_1 \cdots m_{j-1}} \\
&= \frac{j}{m} \sum_{r=1}^{m-1} \sum_{m_1+\ldots+m_{j-1}=r} \frac{1}{m_1 \cdots m_{j-1}}
\end{aligned}$$

which yields the claim. □

Corollary 7.6.10. *We have*

$$\sigma_j(m) = \frac{j!}{m} \sum_{m>m_1>\ldots>m_{j-1}>0} \frac{1}{m_1 \cdots m_{j-1}}.$$

Thus, for instance, $\sigma_2(m) = 2H_{m-1}/m$. From here, we easily re-obtain the evaluations of ω_3 and ω_4 given in Examples 7.6.5 and 7.6.7. To further illustrate Propositions 7.6.8 and 7.6.9, we now compute ρ_5 and ρ_6.

Example 7.6.11 (Evaluation of ρ_5 and ρ_6)**.** From Proposition 7.6.8,

$$\frac{\omega_5(2m)}{m^5} = 10\sigma_1(m)\sigma_4(m) + 20\sigma_2(m)\sigma_3(m).$$

Consequently, for $|\alpha| < 1$,

$$\begin{aligned}
-\rho_5(\alpha) &= \sum_{m=1}^{\infty} \frac{\alpha^{2m}}{(2m)^5}\,\omega_5(2m) \\
&= \frac{10\cdot 4!}{32}\,\mathrm{Li}_{2,1,1,1}(\alpha^2) + \frac{20\cdot 2!\cdot 3!}{32}\left(3\,\mathrm{Li}_{2,1,1,1}(\alpha^2) + \mathrm{Li}_{2,1,2}(\alpha^2) + \mathrm{Li}_{2,2,1}(\alpha^2)\right) \\
&= 30\,\mathrm{Li}_{2,1,1,1}(\alpha^2) + \frac{15}{2}\left(\mathrm{Li}_{2,1,2}(\alpha^2) + \mathrm{Li}_{2,2,1}(\alpha^2)\right). \qquad (7.59)
\end{aligned}$$

Similarly, we have for $|\alpha| < 1$,

$$\begin{aligned}
\rho_6(\alpha) = {}& 180\,\mathrm{Li}_{2,1,1,1,1}(\alpha^2) + 45\left(\mathrm{Li}_{2,1,1,2}(\alpha^2) + \mathrm{Li}_{2,1,2,1}(\alpha^2) + \mathrm{Li}_{2,2,1,1}(\alpha^2)\right) \\
&+ \frac{45}{4}\,\mathrm{Li}_{2,2,2}(\alpha^2). \qquad (7.60)
\end{aligned}$$

From these examples the general pattern, established next, begins to transpire. ♢

In general, ρ_n evaluates as follows:

Theorem 7.6.12 (Evaluation of ρ_n)**.** *For $|\alpha| < 1$ and integers $n \geqslant 2$,*

$$\rho_n(\alpha) = \frac{(-1)^n n!}{4^n} \sum_{w} 4^{\ell(w)}\,\mathrm{Li}_w(\alpha^2)$$

where the sum is over all indices $w = (2, a_2, a_3, \ldots, a_{\ell(w)})$ such that $a_2, a_3, \ldots \in \{1, 2\}$ and $|w| = n$.

Proof. From Proposition 7.6.8 and Corollary 7.6.10 we have

$$\rho_n(\alpha) = \frac{(-1)^n n!}{2^n} \sum_{m=1}^{\infty} \frac{\alpha^{2m}}{m^2} \sum_{j=0}^{n-2} \sum_{\substack{m>m_1>\ldots>m_j>0 \\ m>m_{j+1}>\ldots>m_{n-2}>0}} \frac{1}{m_1 \cdots m_{n-2}}.$$

Combining the right-hand side into harmonic polylogarithms yields

$$\rho_n(\alpha) = \frac{(-1)^n n!}{2^n} \sum_{k=0}^{n-2} \sum_{\substack{a_1,\ldots,a_k\in\{1,2\}\\ a_1+\ldots+a_k=n-2}} 2^{c(a)} \operatorname{Li}_{2,a_1,\ldots,a_k}(\alpha^2)$$

where $c(a)$ is the number of 1s among $a_1, \ldots, a_k$. The claim follows. $\square$

Example 7.6.13 (Special values of ρ_n)**.** Given Theorem 7.6.12, one does not expect to be able to evaluate $\rho_n(\alpha)$ explicitly at most points. Three exceptions are $\alpha = 0$ (which is trivial), $\alpha = 1$, and $\alpha = 1/\sqrt{2}$. For instance we have $\rho_4(1) = \frac{19}{240}\pi^4$ as well as $-\rho_5(1) = \frac{45}{2}\zeta(5) + \frac{5}{4}\zeta(3)$ and $\rho_6(1) = \frac{275}{1344}\pi^6 + \frac{45}{2}\zeta(3)^2$. At $\alpha = 1/\sqrt{2}$ we have

$$\rho_4\left(\frac{1}{\sqrt{2}}\right) = \frac{7}{16}\log^4 2 + \frac{3}{16}\pi^2\log^2 2 - \frac{39}{8}\zeta(3)\log 2 + \frac{13}{192}\pi^4 - 6\operatorname{Li}_4\left(\tfrac{1}{2}\right). \tag{7.61}$$

For $n \geqslant 5$ the expressions are expected to be more complicated. $\Diamond$

7.6.3 Reducing harmonic polylogarithms of low weight

Theorems 7.6.3 and 7.6.12 take us closer to a closed form for $\mu_n(1+x+y)$. As ρ_n are expressible in terms of multiple harmonic polylogarithms of weight n, it remains to supply reductions for those of low weight. Such polylogarithms are reduced [BBBL01] by the use of the differential operators

$$(D_0 f)(x) = x f'(x) \quad \text{and} \quad (D_1 f)(x) = (1-x) f'(x)$$

depending on whether the outer index is '2' or '1'.

1. As was known to Ramanujan, and as studied further in [BB06, §8.1], for $0 < x < 1$,

$$\begin{aligned}\mathrm{Li}_{2,1}(x) = \frac{1}{2}\,\log^2(1-x)\log(x) + \log(1-x)\,\mathrm{Li}_2(1-x)\\ - \mathrm{Li}_3(1-x) + \zeta(3).\end{aligned} \tag{7.62}$$

Equation (7.62), also given in [Lew81], provides a useful expression numerically and symbolically. For future use, we also record the relation, obtainable as in [Lew81, §6.4 & §6.7],

$$\begin{aligned}\mathrm{Re}\ \mathrm{Li}_{2,1}\left(\frac{1}{x}\right) + \mathrm{Li}_{2,1}(x) = \zeta(3) - \frac{1}{6}\log^3 x + \frac{1}{2}\pi^2\log x\\ - \mathrm{Li}_2(x)\log x + \mathrm{Li}_3(x) \qquad \text{for } 0 < x < 1.\end{aligned} \tag{7.63}$$

2. For $\mathrm{Li}_{2,2}$ we work as follows. As $(1-x)\,\mathrm{Li}_{1,2}'(x) = \mathrm{Li}_2\,(x)$, integration yields

$$\begin{aligned}\mathrm{Li}_{1,2}(x) = 2\,\mathrm{Li}_3(1-x) - \log(1-x)\,\mathrm{Li}_2(x) - 2\log(1-x)\,\mathrm{Li}_2(1-x)\\ - \log(1-x)^2\log(x) - 2\zeta(3).\end{aligned} \tag{7.64}$$

Then, since $x\,\mathrm{Li}_{2,2}'(x) = \mathrm{Li}_{1,2}(x)$, on integrating again we obtain $\mathrm{Li}_{2,2}(x)$ in terms of polylogarithms up to order four. We appeal to various formulae in [Lew81, §6.4.4] to arrive at

$$\begin{aligned}\mathrm{Li}_{2,2}(t) = \frac{1}{2}\,\log^2(1-t)\log^2 t - 2\zeta(2)\log(1-t)\log t - 2\zeta(3)\log t - \frac{1}{2}\,\mathrm{Li}_2^2(t)\\ + 2\,\mathrm{Li}_3\,(1-t)\log t - 2\int_0^t \frac{\mathrm{Li}_2\,(x)\log x}{1-x}\,\mathrm{d}x - \int_0^t \frac{\log\,(1-x)\log^2 x}{1-x}\mathrm{d}x.\end{aligned}$$

Expanding the penultimate integral as a series leads to

$$\int_0^t \frac{\mathrm{Li}_2\,(x)\log x}{1-x}\,\mathrm{d}x = \mathrm{Li}_{1,2}(t)\log t - \mathrm{Li}_{2,2}(t).$$

Then, using [Lew81, A3.4 Eq. (12)] to evaluate the remaining integral, we deduce that

$$\begin{aligned}\mathrm{Li}_{2,2}(t) = &-\frac{1}{12}\,\log^4(1-t) + \frac{1}{3}\log^3(1-t)\log t - \zeta(2)\log^2(1-t)\\ &+ 2\log(1-t)\,\mathrm{Li}_3(t) - 2\,\zeta(3)\log(1-t) - 2\,\mathrm{Li}_4(t)\\ &- 2\,\mathrm{Li}_4\left(\frac{t}{t-1}\right) + 2\,\mathrm{Li}_4(1-t) - 2\zeta(4) + \frac{1}{2}\,\mathrm{Li}_2^2(t).\end{aligned} \tag{7.65}$$

3. The form for $\mathrm{Li}_{3,1}(t)$ is obtained in the same way but starting from $\mathrm{Li}_{2,1}(t)$ as given in (7.62). This leads to:

$$2\,\mathrm{Li}_{3,1}(t) + \mathrm{Li}_{2,2}(t) = \frac{1}{2}\,\mathrm{Li}_2^2(t). \tag{7.66}$$

This symmetry result, and its derivative

$$2\,\mathrm{Li}_{2,1}(t) + \mathrm{Li}_{1,2}(t) = \mathrm{Li}_1(t)\,\mathrm{Li}_2(t), \tag{7.67}$$

are also obtained in [Zlo07, Cor. 2 & Cor. 3] by other methods.

4. Since $\mathrm{Li}_{2,1,1}(x) = \int_0^x \mathrm{Li}_{1,1,1}(t)/t\,\mathrm{d}t$ and $\mathrm{Li}_{1,1,1}(x) = \int_0^x \mathrm{Li}_{1,1}(t)/(1-t)\,\mathrm{d}t$, we first compute $\mathrm{Li}_{1,1}(x) = \log^2(1-x)/2$ to find that $\mathrm{Li}_{1,1,1}(x) = -\log^3(1-x)/6$ (the

pattern is clear). Hence

$$\begin{aligned}
\mathrm{Li}_{2,1,1}(x) &= -\frac{1}{6}\int_0^x \log^3(1-t)\frac{\mathrm{d}t}{t} \\
&= \frac{\pi^4}{90} - \frac{1}{6}\log(1-t)^3\log t - \frac{1}{2}\log(1-t)^2\,\mathrm{Li}_2(1-t) \\
&\quad + \log(1-t)\,\mathrm{Li}_3(1-t) - \mathrm{Li}_4(1-t).
\end{aligned} \tag{7.68}$$

5. In general,

$$\mathrm{Li}_{\{1\}^n}(x) = \frac{(-1)^n}{n!}\log(1-x)^n, \tag{7.69}$$

and therefore

$$\begin{aligned}
\mathrm{Li}_{2,\{1\}^{n-1}}(x) &= \frac{(-1)^n}{n!}\int_0^x \log(1-t)^n\frac{\mathrm{d}t}{t} \\
&= \zeta(n+1) - \sum_{m=0}^{n}\frac{(-1)^{n-m}}{(n-m)!}\log(1-x)^{n-m}\,\mathrm{Li}_{m+1}(1-x).
\end{aligned} \tag{7.70}$$

We have, inter alia, provided closed reductions for all multiple polylogarithms of weight less than five. One does not expect such complete results thereafter.

The reductions presented in this section allow us to express ρ_3 and ρ_4 in terms of polylogarithms of depth 1. Equation (7.62) treats ρ_3 while (7.56) leads to

$$\begin{aligned}
\rho_4\left(\alpha^2\right) = {}& 3\left(\mathrm{Li}_3\left(\alpha^2\right) - \zeta(3) + \mathrm{Li}_3\left(1-\alpha^2\right)\right)\log\left(1-\alpha^2\right) - \frac{1}{8}\log^4\left(1-\alpha^2\right) \\
&+ 3\zeta(4) - 3\ \mathrm{Li}_4\left(\frac{-\alpha^2}{1-\alpha^2}\right) - 3\ \mathrm{Li}_4\left(\alpha^2\right) - 3\ \mathrm{Li}_4\left(1-\alpha^2\right) + \frac{3}{4}\mathrm{Li}_2^2\left(1-\alpha^2\right) \\
&- \log\alpha\ \log^3\left(1-\alpha^2\right) - \left(\frac{\pi^2}{4} + 3\,\mathrm{Li}_2\left(1-\alpha^2\right)\right)\log^2\left(1-\alpha^2\right).
\end{aligned} \tag{7.71}$$

7.7 Explicit evaluations of $\mu_n(1+x+y)$ for small n

We now return to the explicit evaluation of the multiple Mahler measures $\mu_k(1+x+y)$. The starting point for this section is the evaluation of $\mu_2(1+x+y)$ from [BS11a] which is reviewed in Section 7.7.1 and was derived alternatively in Theorem 7.5.4. Building on this, we present an informal evaluation of $\mu_3(1+x+y)$ in Section 7.7.2. A conjectural evaluation of $\mu_4(1+x+y)$ is presented in equation (7.107) of the Conclusion.

7.7.1 Evaluation of $\mu_2(1+x+y)$

Theorem 7.7.1 (Evaluation of $\mu_2(1+x+y)$)**.** *We have*

$$\mu_2(1+x+y) = \frac{3}{\pi}\,\mathrm{Ls}_3\left(\frac{2\pi}{3}\right) + \frac{\pi^2}{4}. \tag{7.72}$$

By comparison, Smyth's original result may be written as (see [BS11a])

$$\mu_1(1+x+y) = \frac{3}{2\pi}\,\mathrm{Ls}_2\left(\frac{2\pi}{3}\right) = \frac{1}{\pi}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right). \tag{7.73}$$

We recall from [BS11a] that the evaluation in Theorem 7.7.1 is proceeded by first establishing the following dilogarithmic form.

Proposition 7.7.2 (A dilogarithmic representation)**.** *We have*

(a)

$$\frac{2}{\pi}\int_0^{\pi} \mathrm{Re}\ \mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta = 2\zeta(2), \tag{7.74}$$

(b)

$$\mu_2(1+x+y) = \frac{\pi^2}{36} + \frac{2}{\pi}\int_0^{\pi/6} \mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta. \tag{7.75}$$

We include the proof from [BS11a] as it is instructive for evaluation of $\mu_3(1+x+y)$.

Proof. For (a) we define $\tau(z) := \frac{2}{\pi}\int_0^\pi \mathrm{Li}_2\left(4z\sin^2\theta\right)\mathrm{d}\theta$. This is an analytic function of z. For $|z| < 1/4$ we may use the defining series for Li_2 and expand term by term using Wallis' formula to derive

$$\begin{aligned}\tau(z) &= \frac{2}{\pi}\sum_{n\geqslant 1}\frac{(4z)^n}{n^2}\int_0^\pi \sin^{2n}\theta\,\mathrm{d}\theta = 4z\,{}_4F_3\left(\left.\begin{matrix}1,1,1,\frac{3}{2}\\ 2,2,2\end{matrix}\right|4z\right)\\ &= 4\,\mathrm{Li}_2\left(\frac{1}{2}-\frac{1}{2}\sqrt{1-4z}\right) - 2\log\left(\frac{1}{2}+\frac{1}{2}\sqrt{1-4z}\right)^2.\end{aligned}$$

The final equality can be obtained in *Mathematica* and then verified by differentiation. In particular, the final function provides an analytic continuation from which we obtain $\tau(1) = 2\zeta(2) + 4i\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)$. This yields the assertion.

For (b), commencing much as in [KLO08, Thm. 11], we write

$$\mu_2(1+x+y) = \frac{1}{4\pi^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\mathrm{Re}\,\log\left(1-2\sin(\theta)\mathrm{e}^{i\,\omega}\right)^2\,\mathrm{d}\omega\,\mathrm{d}\theta.$$

We consider the inner integral $\rho(\alpha) := \int_{-\pi}^{\pi}\left(\mathrm{Re}\,\log\left(1-\alpha\,\mathrm{e}^{i\,\omega}\right)\right)^2\,\mathrm{d}\omega$ with $\alpha := 2\sin\theta$. For $|\theta| \leqslant \pi/6$ we directly apply Parseval's identity to obtain

$$\rho(2\sin\theta) = \pi\,\mathrm{Li}_2\left(4\sin^2\theta\right) \tag{7.76}$$

which is equivalent to (7.50) since $\rho(\alpha) = 2\pi\rho_2(\alpha)$. In the remaining case we write

$$\begin{aligned}\rho(\alpha) &= \int_{-\pi}^{\pi}\left\{\log|\alpha| + \mathrm{Re}\,\log\left(1-\alpha^{-1}\,\mathrm{e}^{i\,\omega}\right)\right\}^2\,\mathrm{d}\omega\\ &= 2\pi\,\log^2|\alpha| - 2\log|\alpha|\int_{-\pi}^{\pi}\log\left|1-\alpha^{-1}\,\mathrm{e}^{i\,\omega}\right|\,\mathrm{d}\omega + \pi\,\mathrm{Li}_2\left(\frac{1}{\alpha^2}\right)\\ &= 2\pi\,\log^2|\alpha| + \pi\,\mathrm{Li}_2\left(\frac{1}{\alpha^2}\right),\end{aligned} \tag{7.77}$$

where we have appealed to Parseval's and Jensen's formulae. Thus,

$$\mu_2(1+x+y) = \frac{1}{\pi}\int_0^{\pi/6} \mathrm{Li}_2\left(4\sin^2\theta\right) \mathrm{d}\theta + \frac{1}{\pi}\int_{\pi/6}^{\pi/2} \mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right) \mathrm{d}\theta + \frac{\pi^2}{54}, \tag{7.78}$$

since $\frac{2}{\pi}\int_{\pi/6}^{\pi/2} \log^2\alpha \,\mathrm{d}\theta = \mu(1+x+y_1, 1+x+y_2) = \frac{\pi^2}{54}$. Now, for $\alpha > 1$, the functional equation in [Lew58, A2.1 (6)]

$$\mathrm{Li}_2(\alpha) + \mathrm{Li}_2(1/\alpha) + \frac{1}{2}\log^2\alpha = 2\zeta(2) + i\pi\log\alpha \tag{7.79}$$

gives

$$\int_{\pi/6}^{\pi/2} \left\{\mathrm{Re}\ \mathrm{Li}_2\left(4\sin^2\theta\right) + \mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\right\} \mathrm{d}\theta = \frac{5}{54}\pi^3. \tag{7.80}$$

We then combine (7.74), (7.80) and (7.78) to deduce the desired result (7.75). □

7.7.2 Evaluation of $\mu_3(1+x+y)$

In this section we provide a remarkably concise closed form of $\mu_3(1+x+y)$. We were led to this form by the integer relation algorithm PSLQ [BBG04] (see Example 7.9.2 for some comments on obtaining high precision evaluations), and by considering the evaluation (7.72) of $\mu_2(1+x+y)$.

The details of formalization are formidable — at least by the route chosen here — and so we proceed more informally leaving three conjectural identities.

Conjecture 7.7.3 (Evaluation of $\mu_3(1+x+y)$)**.** *We have*

$$\mu_3(1+x+y) \overset{?[1]}{=} \frac{6}{\pi}\,\mathrm{Ls}_4\left(\frac{2\pi}{3}\right) - \frac{9}{\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right) - \frac{\pi}{4}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) - \frac{13}{2}\zeta(3). \tag{7.81}$$

This evaluation is equivalent to the conjectural identities (7.41) and (7.43).

Proof. We first use Theorem 7.6.3 to write

$$\mu_3(1+x+y) = \frac{2}{\pi}\int_0^{\pi/6} \rho_3(2\sin\theta)\,\mathrm{d}\theta + \frac{2}{\pi}\int_{\pi/6}^{\pi/2} \rho_3\left(\frac{1}{2\sin\theta}\right)\,\mathrm{d}\theta \qquad (7.82)$$
$$+ \frac{3}{\pi}\int_{\pi/6}^{\pi/2} \log(2\sin\theta)\,\mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\,\mathrm{d}\theta - \zeta(3) + \frac{9}{2\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right),$$

on appealing to Examples 7.3.1 and 7.6.4.

Now the functional equation for the dilogarithm (7.79) as used above and knowledge of $\mathrm{Ls}_n\,(\pi/3)$ (see [BS11a, BS11c]) allow us to deduce

$$\frac{3}{\pi}\int_0^{\pi/6} \log(2\sin\theta)\,\mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta + \frac{3}{\pi}\int_0^{\pi/6} \log(2\sin\theta)\,\mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\mathrm{d}\theta$$
$$= \frac{3}{2}\zeta(3) - \frac{\pi}{2}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) + \frac{27}{2\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right), \qquad (7.83)$$
$$\frac{3}{\pi}\int_{\pi/6}^{\pi/2} \log(2\sin\theta)\,\mathrm{Re}\,\mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta + \frac{3}{\pi}\int_{\pi/6}^{\pi/2} \log(2\sin\theta)\,\mathrm{Re}\,\mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\mathrm{d}\theta$$
$$= 3\zeta(3) + \frac{\pi}{2}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) - \frac{27}{2\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right). \qquad (7.84)$$

Moreover, we have

$$\frac{3}{\pi}\left\{\int_0^{\pi/6} + \int_{\pi/6}^{\pi/2}\right\} \log(2\sin\theta)\,\mathrm{Re}\,\mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta \overset{?[2]}{=} \frac{7}{2}\zeta(3) - \pi\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right), \qquad (7.85)$$
$$\frac{3}{\pi}\left\{\int_0^{\pi/6} + \int_{\pi/6}^{\pi/2}\right\} \log(2\sin\theta)\,\mathrm{Re}\,\mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\mathrm{d}\theta \overset{?[2]}{=} \zeta(3) + \pi\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right), \qquad (7.86)$$

which are provable as was (7.74) because, for $|z| < 1/2$, we have

$$\frac{1}{\pi}\int_0^{\pi} \log\left(2\,\sin\frac{\theta}{2}\right)\mathrm{Li}_2\left(4\,z^2\sin^2\frac{\theta}{2}\right)\,\mathrm{d}\theta = \sum_{n=1}^{\infty}\binom{2n}{n}\frac{\sum_{k=1}^{2n}\frac{(-1)^k}{k}}{n^2}\,z^{2n}.$$

(The latter is derivable also from (7.83), (7.84) and (7.85).)

Thence, (7.83), (7.84) and (7.85) together establish that the equality

$$\frac{3}{\pi}\int_{\pi/6}^{\pi/2}\log(2\sin\theta)\ \mathrm{Li}_2\left(\frac{1}{4\sin^2\theta}\right)\mathrm{d}\theta \overset{?[3]}{=} \frac{2}{3}\zeta(3)+\frac{7\pi}{12}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)-\frac{17}{2\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right) \tag{7.87}$$

is true as soon as we establish

$$I_3 := \frac{3}{\pi}\int_0^{\pi/6}\log(2\sin\theta)\,\mathrm{Li}_2\left(4\sin^2\theta\right)\mathrm{d}\theta \overset{?[3]}{=} \frac{7}{6}\,\zeta(3)-\frac{11\pi}{12}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)+5\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right). \tag{7.88}$$

This can, in principle, be achieved by writing the integral as

$$I_3 = \frac{3}{\pi}\sum_{n=1}^{\infty}\frac{1}{n^2}\int_0^1\frac{s^{2n}}{\sqrt{4-s^2}}\log s\,\mathrm{d}s$$

and using the binomial series to arrive at

$$I_3 = -\frac{3}{2\pi}\sum_{m=0}^{\infty}\frac{\binom{2m}{m}}{4^{2m}}\sum_{n=1}^{\infty}\frac{1}{n^2\left(1+2(n+m)\right)^2}. \tag{7.89}$$

This leaves us to deal with the two terms in (7.82) involving ρ_3. These two terms are in turn related by

$$\begin{aligned}\frac{2}{\pi}\int_0^{\pi/6}\mathrm{Li}_{2,1}\left(4\sin^2\theta\right)\mathrm{d}\theta+\frac{2}{\pi}\int_0^{\pi/6}\mathrm{Re}\ \mathrm{Li}_{2,1}\left(\frac{1}{4\sin^2\theta}\right)\mathrm{d}\theta&\\ =\frac{1}{9}\left\{\zeta(3)-\pi\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)+\frac{6}{\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right)\right\},&\end{aligned} \tag{7.90}$$

as we see by integrating (7.63). Likewise,

$$\begin{aligned}\frac{2}{\pi}\int_{\pi/6}^{\pi/2}\mathrm{Re}\ \mathrm{Li}_{2,1}\left(4\sin^2\theta\right)\mathrm{d}\theta+\frac{2}{\pi}\int_{\pi/6}^{\pi/2}\mathrm{Li}_{2,1}\left(\frac{1}{4\sin^2\theta}\right)\mathrm{d}\theta&\\ =\frac{1}{9}\left\{2\zeta(3)-5\pi\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)-\frac{6}{\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right)\right\}.&\end{aligned} \tag{7.91}$$

Also, using (7.62) we arrive at

$$\frac{2}{\pi}\int_0^{\pi/6} \mathrm{Li}_{2,1}\left(4\sin^2\theta\right)\mathrm{d}\theta = \frac{20}{27}\zeta(3) - \frac{8\pi}{27}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) + \frac{4}{9\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right) + \frac{1}{\pi}\int_0^{\pi/3} \log^2\left(1-4\sin^2\frac{\theta}{2}\right)\log\left(2\sin\frac{\theta}{2}\right)\mathrm{d}\theta, \tag{7.92}$$

and

$$\frac{2}{\pi}\int_0^{\pi/2} \mathrm{Re}\ \mathrm{Li}_{2,1}\left(4\sin^2\theta\right)\mathrm{d}\theta = \frac{1}{3}\zeta(3) - \frac{2\pi}{3}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right). \tag{7.93}$$

We may now establish — from (7.87), (7.90), (7.91), (7.92), (7.93) and (7.82) — that

$$\mu_3(1+x+y) = \frac{43}{18}\zeta(3) - \frac{47\pi}{36}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) - \frac{13}{3\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right) + \frac{2}{\pi}\int_0^{\pi/3} \log^2\left(1-4\sin^2\frac{\theta}{2}\right)\log\left(2\sin\frac{\theta}{2}\right)\mathrm{d}\theta. \tag{7.94}$$

Hence, to prove (7.81) we are reduced to verifying that

$$-\frac{1}{\pi}\,\mathrm{Ls}_4\left(\frac{2\pi}{3}\right) \overset{?[4]}{=} -\frac{37}{54}\zeta(3) + \frac{7\pi}{27}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) - \frac{7}{9\pi}\,\mathrm{Cl}_4\left(\frac{\pi}{3}\right) + \frac{1}{2\pi}\int_0^{\pi/3} \log^2\left(1-4\sin^2\frac{\theta}{2}\right)\log\left(2\sin\frac{\theta}{2}\right)\mathrm{d}\theta. \tag{7.95}$$

which completes the evaluation. $\square$

Remark 7.7.4. By noting that, for integers $n \geqslant 2$,

$$\mathrm{Cl}_n\left(\frac{\pi}{3}\right) = \left(\frac{1}{2^{n-1}} + (-1)^n\right)\mathrm{Cl}_n\left(\frac{2\pi}{3}\right),$$

the arguments of the Clausen functions in the evaluation (7.81) of $\mu_3(1+x+y)$ may be transformed to $\frac{2\pi}{3}$.

Many further variations are possible. For instance, it follows from [BS11c] that

$$\mathrm{Ls}_4\left(\frac{2\pi}{3}\right) = \frac{31}{18}\,\pi\zeta(3) + \frac{\pi^2}{12}\,\mathrm{Cl}_2\left(\frac{2\pi}{3}\right) - \frac{3}{2}\,\mathrm{Cl}_4\left(\frac{2\pi}{3}\right) + 6\,\mathrm{Cl}_{2,1,1}\left(\frac{2\pi}{3}\right) \tag{7.96}$$

in terms of multi Clausen values. ♢

7.8 Proofs of two conjectures of Boyd

We now use log-sine integrals to recapture the following evaluations conjectured by Boyd in 1998 and first proven in [Tou08] using *Bloch-Wigner* logarithms. Below, L_{-n} denotes a primitive L-series and G is Catalan's constant.

Theorem 7.8.1 (Two quadratic evaluations)**.** *We have*

$$\mu(y^2(x+1)^2 + y(x^2+6x+1) + (x+1)^2) = \frac{16}{3\pi}\,\mathrm{L}_{-4}(2) = \frac{16}{3\pi}\,\mathrm{G}, \tag{7.97}$$

as well as

$$\mu(y^2(x+1)^2 + y(x^2-10x+1) + (x+1)^2) = \frac{5\sqrt{3}}{\pi}\,\mathrm{L}_{-3}(2) = \frac{20}{3\,\pi}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right). \tag{7.98}$$

Proof. Let $P_c = y^2(x+1)^2 + y(x^2+2cx+1) + (x+1)^2$ and $\mu_c = \mu(P_c)$ for a real variable c. We set $x = \mathrm{e}^{2\pi i t}$, $y = \mathrm{e}^{2\pi i u}$ and note that

$$\begin{aligned}
|P_c| &= |(x+1)^2(y^2+y+1) + 2(c-1)xy| \\
&= \left|(x+x^{-1}+2)(y+1+y^{-1}) + 2(c-1)\right| \\
&= |2(\cos(2\pi t)+1)(2\cos(2\pi u)+1) + 2(c-1)| \\
&= 2\,|c + 2\cos(2\pi u) + (1+2\cos(2\pi u))\cos(2\pi t)|.
\end{aligned}$$

It is known that (see [GR80, §4.224, Ex. 9]), for real a, b with $|a| \geqslant |b| > 0$,

$$\int_0^1 \log|2a + 2b\cos(2\pi\theta)|\,\mathrm{d}\theta = \log\left(|a| + \sqrt{a^2 - b^2}\right). \tag{7.99}$$

Applying this, with $a = c + 2\cos(2\pi u)$ and $b = 1 + 2\cos(2\pi u))$ to $\int_0^1 |P_c|\,\mathrm{d}t$, we get

$$\mu_c = \int_0^1 \log\left|c + 2\cos(2\pi u) + \sqrt{(c^2-1) + 4(c-1)\cos(2\pi u)}\right|\,\mathrm{d}u. \tag{7.100}$$

If $c^2 - 1 = \pm 4(c-1)$, that is if $c = 3$ or $c = -5$, then the surd is a perfect square and also $|a| \geqslant |b|$.

(a) When $c = 3$ for (7.97), by symmetry, after factorization we obtain

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

as required, since $\mathrm{Ls}_2\left(\frac{3\pi}{2}\right) = -\,\mathrm{Ls}_2\left(\frac{\pi}{2}\right) = \mathrm{L}_{-4}(2)$, which is Catalan's constant G.

(b) When $c = -5$ for (7.98), we likewise obtain

$$\begin{aligned}
\mu_{-5} &= \frac{2}{\pi}\int_0^\pi \log\left(\sqrt{3} + 2\sin\theta\right)\mathrm{d}\theta = \frac{2}{\pi}\int_{\pi/3}^{4\pi/3}\log\left(\sqrt{3} + 2\sin\left(\theta - \frac{\pi}{3}\right)\right)\mathrm{d}\theta \\
&= \frac{2}{\pi}\int_{\pi/3}^{4\pi/3}\left\{\log 2\left(\sin\frac{\theta}{2}\right) + \log 2\left(\sin\frac{\theta + \frac{\pi}{3}}{2}\right)\right\}\mathrm{d}\theta \\
&= \frac{2}{\pi}\int_{\pi/3}^{4\pi/3}\log 2\left(\sin\frac{\theta}{2}\right)\mathrm{d}\theta + \frac{2}{\pi}\int_{2\pi/3}^{5\pi/3}\log 2\left(\sin\frac{\theta}{2}\right)\mathrm{d}\theta \\
&= \frac{4}{\pi}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right) - \frac{4}{\pi}\,\mathrm{Cl}_2\left(\frac{4\pi}{3}\right) = \frac{20}{3\pi}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right),
\end{aligned}$$

since $\mathrm{Cl}_2\left(\frac{4\pi}{3}\right) = -\frac{2}{3}\,\mathrm{Cl}_2\left(\frac{\pi}{3}\right)$ and so we are done. □

When $c = 1$ the cosine in the surd disappears, and we obtain $\mu_1 = 0$, which is trivial as in this case the polynomial factorizes as $(1+x)^2(1+y+y^2)$. For $c = -1$ we are able, with some care, to directly integrate (7.100) and so to obtain an apparently new Mahler measure:

Theorem 7.8.2. *We have*

$$\begin{aligned} \mu_{-1} &= \mu\left((x+1)^2(y^2+y+1) - 2xy\right) \\ &= \frac{1}{\pi}\left\{\frac{1}{2}B\left(\frac{1}{4},\frac{1}{4}\right){}_3F_2\left(\left.\begin{matrix}\frac{1}{4},\frac{1}{4},1\\ \frac{3}{4},\frac{5}{4}\end{matrix}\right|\frac{1}{4}\right) - \frac{1}{6}B\left(\frac{3}{4},\frac{3}{4}\right){}_3F_2\left(\left.\begin{matrix}\frac{3}{4},\frac{3}{4},1\\ \frac{5}{4},\frac{7}{4}\end{matrix}\right|\frac{1}{4}\right)\right\}. \end{aligned} \tag{7.101}$$

Here, $B(s,t) = \frac{\Gamma(s)\Gamma(t)}{\Gamma(s+t)}$ *denotes the Euler beta function.*

We observe that an alternative form of μ_{-1} is given by

$$\mu_{-1} = \mu\left(\left(x + 1/x + 2\sqrt{1/x}\right)(y + 1/y + 1) - 2\right).$$

Remark 7.8.3. Equation (7.99) may be applied to other conjectured Mahler measures. For instance, $\mu(1 + x + y + 1/x + 1/y) = .25133043371325\ldots$ was conjectured by Deninger [Fin05] to evaluate in L-series terms as

$$\mu(1 + x + y + 1/x + 1/y) = 15\sum_{n=1}^{\infty}\frac{a_n}{n^2}, \tag{7.102}$$

where $\sum_{n=1}^{\infty} a_n q^n = \eta(q)\eta(q^3)\eta(q^5)\eta(q^{15})$. Here η is the *Dirichlet eta-function*:

$$\eta(q) := q^{1/24}\prod_{n=1}^{\infty}(1-q^n) = q^{1/24}\sum_{n=-\infty}^{\infty}(-1)^n q^{n(3n+1)/2}. \tag{7.103}$$

This has recently been proven in [RZ11].

Application of (7.99) shows that

$$\mu(1+x+y+1/x+1/y) = \frac{1}{\pi}\int_0^{\pi/3} \log\left(\frac{1+2\cos\theta}{2} + \sqrt{\left(\frac{1+2\cos\theta}{2}\right)^2 - 1}\right) \mathrm{d}\theta,$$

but the surd remains an obstacle to a direct evaluation. ◊

7.9 Conclusion

To recapitulate, $\mu_k(1+x+y) = W_3^{(k)}(0)$ has been evaluated in terms of log-sine integrals for $1 \leqslant k \leqslant 3$. Namely,

$$\mu_1(1+x+y) = \frac{3}{2\pi}\operatorname{Ls}_2\left(\frac{2\pi}{3}\right), \tag{7.104}$$

$$\mu_2(1+x+y) = \frac{3}{\pi}\operatorname{Ls}_3\left(\frac{2\pi}{3}\right) + \frac{\pi^2}{4}, \tag{7.105}$$

$$\mu_3(1+x+y) \overset{?[1]}{=} \frac{6}{\pi}\operatorname{Ls}_4\left(\frac{2\pi}{3}\right) - \frac{9}{\pi}\operatorname{Cl}_4\left(\frac{\pi}{3}\right) - \frac{\pi}{4}\operatorname{Cl}_2\left(\frac{\pi}{3}\right) - \frac{13}{2}\zeta(3). \tag{7.106}$$

Hence it is reasonable to ask whether $\mu_4(1+x+y)$ and higher Mahler measures have evaluations in similar terms.

Example 7.9.1. In the case of $\mu_4(1+x+y)$, numerical experiments suggest that

$$\begin{aligned}\pi\mu_4(1+x+y) \overset{?[5]}{=} {}& 12\operatorname{Ls}_5\left(\frac{2\pi}{3}\right) - \frac{49}{3}\operatorname{Ls}_5\left(\frac{\pi}{3}\right) + 81\operatorname{Gl}_{4,1}\left(\frac{2\pi}{3}\right) \\ &+ 3\pi^2\operatorname{Gl}_{2,1}\left(\frac{2\pi}{3}\right) + 2\zeta(3)\operatorname{Cl}_2\left(\frac{\pi}{3}\right) + \pi\operatorname{Cl}_2\left(\frac{\pi}{3}\right)^2 - \frac{29}{90}\pi^5\end{aligned} \tag{7.107}$$

while the higher Mahler measure $\mu_5(1+x+y)$ does not appear to have an evaluation in terms of generalized Glaisher and Clausen values only. ◊

We close with numerical values for these quantities.

Example 7.9.2. By computing higher-order finite differences in the right-hand side of (7.21) we have obtained values for $\mu_n(1+x+y)$ to several thousand digits. To confirm these values we have evaluated the double-integral (7.23) to about 250 digits for all $n \leqslant 8$. These are the results for $\mu_k := \mu_k(1+x+y)$ to fifty digits:

$$\mu_2 = 0.41929927830117445534618570174886146566170299117521, \tag{7.108}$$

$$\mu_3 = 0.13072798584098927059592540295887788768895327503289, \tag{7.109}$$

$$\mu_4 = 0.52153569858138778267996782141801173128244973155094, \tag{7.110}$$

$$\mu_5 = -0.46811264825699083401802243892432823881642492433794. \tag{7.111}$$

These values will allow a reader to confirm many of our results numerically. $\Diamond$

Chapter 8

Ramanujan's Master Theorem

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[AEG+11] *Ramanujan's Master Theorem*
(with Tewodros Amdeberhan, Ivan Gonzalez, Marshall Harrison, Victor H. Moll)
to appear in The Ramanujan Journal

Abstract S. Ramanujan introduced a technique, known as Ramanujan's Master Theorem, which provides an explicit expression for the Mellin transform of a function in terms of the analytic continuation of its Taylor coefficients. The history and proof of this result are reviewed, and a variety of applications is presented. Finally, a multi-dimensional extension of Ramanujan's Master Theorem is discussed.

8.1 Introduction

Ramanujan's Master Theorem refers to the formal identity

$$\int_0^\infty x^{s-1} \left\{ \lambda(0) - \frac{x}{1!}\lambda(1) + \frac{x^2}{2!}\lambda(2) - \cdots \right\} \mathrm{d}x = \Gamma(s)\lambda(-s) \tag{8.1}$$

stated by S. Ramanujan's in his *Quarterly Reports* [Ber85, p. 298]. It was widely used by him as a tool in computing definite integrals and infinite series. In fact, as

G. H. Hardy puts it in [Har78], he “was particularly fond of them [(8.1) and (8.6)], and used them as one of his commonest tools.”

The goal of this semi-expository paper is to discuss the history of (8.1) and to describe a selection of applications of this technique. Section 8.2 discusses evidence that (8.1) was nearly discovered as early as 1874 by J. W. L. Glaisher and J. O’Kinealy. Section 8.3 briefly outlines Hardy’s proof of Ramanujan’s Master Theorem. The critical issue is the extension of the function λ from $\mathbb{N}$ to $\mathbb{C}$. Section 8.4 presents the evaluation of a collection of definite integrals with most of the examples coming from the classical table [GR80]. Further examples of definite integrals are given in Section 8.8 which collects integrals derived from classical polynomials.

Section 8.5 is a recollection on the evaluation of the quartic integral

$$N_{0,4}(a;m) = \int_0^\infty \frac{\mathrm{d}x}{(x^4+2ax^2+1)^{m+1}}. \tag{8.2}$$

This section provides a personal historical context: it was the evaluation of (8.2) that lead one of the authors to (8.1).

Sections 8.6 and 8.9 outline the use of Ramanujan’s Master Theorem to ongoing research projects: Section 8.6 deals with an integral related to the distance traveled by a uniform random walk in a fixed number of steps; finally, Section 8.9 presents a multi-dimensional version of the main theorem that has appeared in the context of Feynman diagrams.

The use of Ramanujan’s Master Theorem has been restricted here mostly to the evaluation of definite integrals. Many other applications appear in the literature. For instance, Ramanujan himself employed it to derive various expansions: the two examples given in [Har78, 11.9] are the expansion of e^{-ax} in powers of $x\mathrm{e}^{bx}$ as well as an expansion of the powers x^r of a root of $aqx^p + x^q = 1$ in terms of powers of a.

8.2 History

The first integral theorem in the spirit of Ramanujan's Master Theorem appears to have been given by Glaisher in 1874, [Gla74b]:

$$\int_0^\infty \left(a_0 - a_1 x^2 + a_2 x^4 - \ldots\right) \, \mathrm{d}x = \frac{\pi}{2} a_{-\frac{1}{2}}. \tag{8.3}$$

Glaisher writes, "of course, a_n being only defined for n a positive integer, $a_{-\frac{1}{2}}$ is without meaning. But in cases where a_n involves factorials, there is a strong presumption, derived from experience in similar questions, that the formula will give correct results if the continuity of the terms is preserved by the substitution of gamma functions for the factorials. This I have found to be true in every case to which I have applied (8.3)."

Glaisher in [Gla74b] formally obtained (8.3) by integrating term-by-term the identity

$$a_0 - a_1 x^2 + a_2 x^4 - \cdots = \frac{a_0}{1+x^2} - \Delta a_0 \frac{x^2}{(1+x^2)^2} + \Delta^2 a_0 \frac{x^4}{(1+x^2)^3} - \cdots . \tag{8.4}$$

Here Δ is the forward-difference operator defined by $\Delta a_n = a_{n+1} - a_n$.

Glaisher's argument, published in July 1874, was picked up in October of the same year by O'Kinealy who critically simplified it in [O'K74]. Employing the forward-shift operator E defined by $E \cdot \lambda(n) = \lambda(n+1)$, O'Kinealy writes the left-hand side of (8.4) as $\frac{1}{1+x^2 E} \cdot a_0$ which he then integrates treating E as a number to obtain

$$\frac{\pi}{2} E^{-1/2} \cdot a_0 = \frac{\pi}{2} a_{-\frac{1}{2}},$$

thus arriving at the identity (8.3). O'Kinealy, [O'K74], remarks that "it is evident that there are numerous theorems of the same kind". As an example, he proposes integrating $\cos(xE) \cdot a_0$ and $\sin(xE) \cdot a_0$.

O'Kinealy's improvements are emphatically received by Glaisher in a short letter [Gla74a] to the editors in which he remarks that he had examined O'Kinealy's work and that, "after developing the method so far as to include these formulae and several others, I communicated it, with the examples, to Professor Cayley, in a letter on the 22nd or 23rd of July, which gave rise to a short correspondence between us on the matter at the end of July. My only reason for wishing to mention this at once is that otherwise, as I hope soon to be able to return to the subject and somewhat develop the principle, which is to a certain extent novel, it might be thought at some future time that I had availed myself of Mr. O'Kinealy's idea without proper acknowledgement."

Unfortunately, no further work seems to have appeared along these lines so that one can only speculate as to what Glaisher and Cayley have figured out. It is not unreasonable to guess that they might very well have developed an idea somewhat similar to Ramanujan's Master Theorem (8.1). In fact, just slightly generalizing O'Kinealy's argument is enough to formally obtain (8.1). This is shown next.

Formal proof of (8.1).

$$\begin{aligned}
\int_0^\infty x^{s-1} \sum_{n=0}^\infty \frac{(-1)^n}{n!} \lambda(n) x^n \,\mathrm{d}x &= \int_0^\infty x^{s-1} \sum_{n=0}^\infty \frac{(-1)^n}{n!} E^n x^n \,\mathrm{d}x \cdot \lambda(0) \\
&= \int_0^\infty x^{s-1} \mathrm{e}^{-Ex} \,\mathrm{d}x \cdot \lambda(0) \\
&= \frac{\Gamma(s)}{E^s} \cdot \lambda(0) \\
&= \Gamma(s) \lambda(-s)
\end{aligned}$$

where in the penultimate step the integral representation

$$\Gamma(s) = \int_0^\infty x^{s-1} e^{-x}\, dx \tag{8.5}$$

of the gamma function was employed and the operator E treated as a number. It is this step which renders the proof formal: clearly the coefficient function $\lambda(n)$ needs to satisfy certain conditions for the result to be valid. This will be discussed in Section 8.3. $\square$

The identity

$$\int_0^\infty x^{s-1} \left\{ \varphi(0) - x\varphi(1) + x^2\varphi(2) - \cdots \right\} dx = \frac{\pi}{\sin s\pi}\varphi(-s), \tag{8.6}$$

is given by Ramanujan alongside (8.1) (see [Ber85]). The formulations are equivalent: the relation $\varphi(n) = \lambda(n)/\Gamma(n+1)$ converts (8.6) into (8.1).

The integral theorem (8.3) also appears in the text [Edw22] as Exercise 7 on Chapter XXVI. It is attributed there to Glaisher. The exercise asks to show (8.3) and to "apply this theorem to find $\int_0^\infty \frac{\sin ax}{x}\, dx$."

The argument that Ramanujan gives for (8.1) appears in Hardy [Har78] where the author demonstrates that, while the argument can be made rigorous in certain cases, it usually leads to false intermediate formulae which "excludes practically all of Ramanujan's examples".

A rigorous proof of (8.1) and its special case (8.3) was given in Chapter XI of [Har78]. This text is based on a series of lectures on Ramanujan's work given in the Fall semester of 1936 at Harvard University.

8.3 Rigorous treatment of the Master Theorem

The proof of Ramanujan's Master Theorem provided by Hardy in [Har78] employs Cauchy's residue theorem as well as the well-known Mellin inversion formula which is recalled next followed by an outline of the proof.

Theorem 8.3.1 (Mellin inversion formula). *Assume that $F(s)$ is analytic in the strip $a < \operatorname{Re}\, s < b$ and define f by*

$$f(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} F(s) x^{-s} \, \mathrm{d}s.$$

If this integral converges absolutely and uniformly for $c \in (a,b)$ then

$$F(s) = \int_0^\infty x^{s-1} f(x) \, \mathrm{d}x.$$

Theorem 8.3.2 (Ramanujan's Master Theorem). *Let $\varphi(z)$ be an analytic (single-valued) function, defined on a half-plane*

$$H(\delta) = \{z \in \mathbb{C} : \operatorname{Re}\, z \geq -\delta\} \tag{8.7}$$

for some $0 < \delta < 1$. Suppose that, for some $A < \pi$, φ satisfies the growth condition

$$|\varphi(v + iw)| < C\mathrm{e}^{Pv + A|w|} \tag{8.8}$$

for all $z = v + iw \in H(\delta)$. Then (8.6) holds for all $0 < \operatorname{Re}\, s < \delta$, that is

$$\int_0^\infty x^{s-1} \left\{ \varphi(0) - x\varphi(1) + x^2\varphi(2) - \cdots \right\} \, \mathrm{d}x = \frac{\pi}{\sin s\pi} \varphi(-s). \tag{8.9}$$

Proof. Let $0 < x < \mathrm{e}^{-P}$. The growth conditions show that the series

$$\Phi(x) = \varphi(0) - x\varphi(1) + x^2\varphi(2) - \cdots$$

converges. The residue theorem yields

$$\Phi(x) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+\infty} \frac{\pi}{\sin \pi s}\varphi(-s)x^{-s}\,\mathrm{d}s \tag{8.10}$$

for any $0 < c < \delta$. Observe that $\pi/\sin(\pi s)$ has poles at $s = -n$ for $n = 0, 1, 2, \ldots$ with residue $(-1)^n$. The integral in (8.10) converges absolutely and uniformly for $c \in (a, b)$ for any $0 < a < b < \delta$. The claim now follows from Theorem 8.3.1. $\square$

Remark 8.3.3. The conversion $\varphi(u) = \lambda(u)/\Gamma(u+1)$ establishes Ramanujan's Master Theorem in the form (8.1). The condition $\delta < 1$ ensures convergence of the integral in (8.9). Analytic continuation may be employed to validate (8.9) to a larger strip in which the integral converges. See also Section 8.7.

8.4 A collection of elementary examples

This section contains a collection of definite integrals that can be evaluated directly from Ramanujan's Master Theorem 8.3.2. For the convenience of the reader, the main theorem in the form (8.1) is reproduced below. Its hypotheses are described in Section 8.3.

Theorem 8.4.1. *Assume f admits an expansion of the form*

$$f(x) = \sum_{k=0}^{\infty} \frac{\lambda(k)}{k!}(-x)^k. \tag{8.11}$$

Then, the Mellin transform of f is given by

$$\int_0^\infty x^{s-1} f(x)\, \mathrm{d}x = \Gamma(s)\lambda(-s). \tag{8.12}$$

Example 8.4.2. Instances of series expansions involving factorials are particularly well-suited for the application of Ramanujan's Master Theorem. To illustrate this fact, use the binomial theorem for $a > 0$ in the form

$$(1+x)^{-a} = \sum_{k=0}^{\infty} \binom{k+a-1}{k} (-x)^k = \sum_{k=0}^{\infty} \frac{\Gamma(k+a)}{\Gamma(a)} \frac{(-x)^k}{k!}. \tag{8.13}$$

Ramanujan's Master Theorem (8.1), with $\lambda(k) = \Gamma(a+k)/\Gamma(a)$, then yields

$$\int_0^\infty \frac{x^{s-1}\, dx}{(1+x)^a} = \frac{\Gamma(s)\Gamma(a-s)}{\Gamma(a)} = B(s, a-s) \tag{8.14}$$

where B is the beta integral.

Example 8.4.3. Several of the functions appearing in this paper are special cases of the hypergeometric function

$${}_pF_q(\mathbf{c}; \mathbf{d}; -x) = \sum_{k=0}^{\infty} \frac{(c_1)_k\, (c_2)_k \cdots (c_p)_k}{(d_1)_k\, (d_2)_k \cdots (d_q)_k} \frac{(-x)^k}{k!} \tag{8.15}$$

where $\mathbf{c} = (c_1, \ldots, c_p)$, $\mathbf{d} = (d_1, \ldots, d_q)$, and $(a)_k = a(a+1)\cdots(a+k-1)$ denotes the rising factorial. To apply Ramanujan's Master Theorem, write $(a)_k = \Gamma(a+k)/\Gamma(a)$. The result is the standard evaluation

$$\int_0^\infty x^{s-1}{}_pF_q(\mathbf{c}; \mathbf{d}; -x)\, \mathrm{d}x = \Gamma(s) \frac{\Gamma(c_1 - s)\, \cdots \Gamma(c_p - s)\Gamma(d_1) \cdots \Gamma(d_q)}{\Gamma(c_1)\, \cdots \Gamma(c_p)\Gamma(d_1 - s) \cdots \Gamma(d_q - s)}, \tag{8.16}$$

which appears as Entry 7.511 in [GR80].

Example 8.4.4. The Bessel function $J_\nu(x)$ admits the hypergeometric representation

$$J_\nu(x) = \frac{1}{\Gamma(\nu+1)} \frac{x^\nu}{2^\nu} \, {}_0F_1\left(-; \nu+1; -\frac{x^2}{4}\right). \tag{8.17}$$

Its Mellin transform is therefore obtained from (8.16) as

$$\int_0^\infty x^{s-1} J_\nu(x)\, \mathrm{d}x = \frac{2^{s-1}\Gamma\left(\frac{s+\nu}{2}\right)}{\Gamma\left(\frac{\nu-s}{2}+1\right)}. \tag{8.18}$$

This formula appears as 6.561.14 in [GR80].

Example 8.4.5. The expansion

$$\frac{\cos(t \tan^{-1}\sqrt{x})}{(1+x)^{t/2}} = \sum_{k=0}^\infty \frac{\Gamma(t+2k)\,\Gamma(k+1)}{\Gamma(t)\,\Gamma(2k+1)} \frac{(-x)^k}{k!}.$$

was established in [BEM03] in the process of evaluating of a class of definite integrals (alternatively, as pointed out by the referee, the expansion may be deduced hypergeometricly; in fact, the conversion is done automatically by `Mathematica` 7 upon expressing the series as a hypergeometric function). A direct application of Ramanujan's Master Theorem yields

$$\int_0^\infty x^{\nu-1} \frac{\cos(2t \tan^{-1}\sqrt{x})}{(1+x)^t}\, \mathrm{d}x = \frac{\Gamma(2t-2\nu)\,\Gamma(1-\nu)\,\Gamma(\nu)}{\Gamma(2t)\,\Gamma(1-2\nu)},$$

and $x = \tan^2\theta$ gives

$$\int_0^{\pi/2} \sin^\mu\theta \cos^{2t-\mu}\theta \cos(2t\theta)\, \mathrm{d}\theta = \frac{\pi\Gamma(2t-\mu-1)}{2\sin(\pi\mu/2)\,\Gamma(2t)\Gamma(-\mu)}. \tag{8.19}$$

Similarly, the expansion

$$\frac{\sin(2t \tan^{-1}\sqrt{x})}{\sqrt{x}(1+x)^t} = \sum_{k=0}^\infty \frac{\Gamma(2t+2k+1)\,\Gamma(k+1)}{\Gamma(2t)\Gamma(2k+2)} \frac{(-x)^k}{k!}$$

produces

$$\int_0^{\pi/2} \sin^{\mu-1}\theta \cos^{2t-\mu}\theta \, \sin(2t\theta)\, \mathrm{d}\theta = \frac{\pi\Gamma(2t-\mu)}{2\sin(\pi\mu/2)\Gamma(2t)\Gamma(1-\mu)}. \tag{8.20}$$

Example 8.4.6. The Mellin transform of the function $\log(1+x)/(1+x)$ is obtained from the expansion

$$\frac{\log(1+x)}{1+x} = -\sum_{k=1}^{\infty} H_k(-x)^k, \tag{8.21}$$

where $H_k = 1 + \frac{1}{2} + \cdots + \frac{1}{k}$ is the kth harmonic number. The analytic continuation of the harmonic numbers, required for an application of Ramanujan's Master Theorem, is achieved by the relation

$$H_k = \gamma + \psi(k+1), \tag{8.22}$$

where $\psi(x) = \Gamma'(x)/\Gamma(x)$ is the digamma function and $\gamma = -\Gamma'(1)$ is the Euler constant. The expansion (8.21) and Ramanujan's Master Theorem now give

$$\int_0^{\infty} \frac{x^{\nu-1}}{1+x} \log(1+x)\, \mathrm{d}x = -\frac{\pi}{\sin \pi\nu} \left(\gamma + \psi(1-\nu)\right). \tag{8.23}$$

The special case $\nu = \frac{1}{2}$ produces the logarithmic integral

$$\int_0^{\infty} \frac{\log(1+t^2)}{1+t^2}\, \mathrm{d}t = \pi \log 2 \tag{8.24}$$

which is equivalent to the classic evaluation

$$\int_0^{\pi/2} \log \sin x \, \mathrm{d}x = -\frac{\pi}{2} \log 2 \tag{8.25}$$

given by Euler.

Example 8.4.7. The infinite product representation of the gamma function

$$\Gamma(x) = \frac{e^{-\gamma x}}{x} \prod_{n=1}^{\infty} \left(1 + \frac{x}{n}\right)^{-1} e^{x/n} \tag{8.26}$$

is equivalent to the expansion

$$\log \Gamma(1+x) = -\gamma x + \sum_{k=2}^{\infty} \frac{\zeta(k)}{k} (-x)^k. \tag{8.27}$$

Hence Ramanujan's Master Theorem implies

$$\int_0^\infty x^{\nu-1} \frac{\gamma x + \log \Gamma(1+x)}{x^2} \, dx = \frac{\pi}{\sin \pi\nu} \frac{\zeta(2-\nu)}{2-\nu}, \tag{8.28}$$

valid for $0 < \nu < 1$.

8.5 A quartic integral

The authors' first encounter with Ramanujan's Master Theorem occured while evaluating the quartic integral

$$N_{0,4}(a;m) = \int_0^\infty \frac{dx}{(x^4 + 2ax^2 + 1)^{m+1}}. \tag{8.29}$$

The goal was to provide a proof of the experimental observation that

$$N_{0,4}(a;m) = \frac{\pi}{2^{m+3/2}\,(a+1)^{m+1/2}} P_m(a), \tag{8.30}$$

where

$$P_m(a) = 2^{-2m} \sum_{k=0}^{m} 2^k \binom{2m-2k}{m-k} \binom{m+k}{m} (a+1)^k. \tag{8.31}$$

The reader will find in [AM09] a variety of proofs of this identity, but it was Ramanujan's Master Theorem that was key to the first proof of (8.30). This proof is outlined next.

The initial observation is that the double square root function $\sqrt{a+\sqrt{1+c}}$ satisfies the unexpected relation

$$\frac{\mathrm{d}}{\mathrm{d}c}\sqrt{a+\sqrt{1+c}} = \frac{1}{\pi\sqrt{2}}\int_0^\infty \frac{dx}{x^4+2ax^2+1+c}. \tag{8.32}$$

This leads naturally to the Taylor series expansion

$$\sqrt{a+\sqrt{1+c}} = \sqrt{a+1} + \frac{1}{\pi\sqrt{2}}\sum_{k=1}^{\infty}\frac{(-1)^{k-1}}{k}N_{0,4}(a;k-1)c^k. \tag{8.33}$$

Thus, in terms of

$$\lambda(k) = -\frac{(k-1)!}{\pi\sqrt{2}}N_{0,4}(a;k-1), \tag{8.34}$$

Ramanujan's Master Theorem implies that

$$\Gamma(s)\lambda(-s) = \int_0^\infty c^{s-1}\sqrt{a+\sqrt{1+c}}\,\mathrm{d}c. \tag{8.35}$$

The next ingredient emerges from a direct differentiation of the integral $N_{0,4}$:

$$\left(\frac{\mathrm{d}}{\mathrm{d}a}\right)^j N_{0,4}(a;k-1) = \frac{(-1)^j 2^j (k+j-1)!}{(k-1)!}\int_0^\infty \frac{x^{4k+2j-2}\,\mathrm{d}x}{(x^4+2ax^2+1)^{k+j}}$$

Note that the integral on the right-hand side can be expressed in terms of $N_{0,4}$ if $j = 1-2k$. In this case, the formal relation

$$\left(\frac{\mathrm{d}}{\mathrm{d}a}\right)^{1-2k}\lambda(k) = (-2)^{1-2k}\lambda(1-k) \tag{8.36}$$

is obtained. This may be rewritten as

$$\lambda(m+1) = \left(-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}a}\right)^{2m+1} \lambda(-m) \tag{8.37}$$

and relates the quartic integral $N_{0,4}(a;m)$, as a function in m, to its analytic continuation appearing in (8.35). Combining (8.37) and (8.35) one arrives at

$$\begin{aligned} N_{0,4}(a;m) &= \frac{\pi\sqrt{2}}{2^{2m+1}(m-1)!m!}\left(\frac{\mathrm{d}}{\mathrm{d}a}\right)^{2m+1}\int_0^\infty c^{m-1}\sqrt{a+\sqrt{1+c}}\,\mathrm{d}c \\ &= \frac{m\pi\sqrt{2}}{2^{6m+2}}\binom{4m}{2m}\binom{2m}{m}\int_0^\infty \frac{c^{m-1}\,\mathrm{d}c}{(a+\sqrt{1+c})^{2m+1/2}}. \end{aligned} \tag{8.38}$$

The substitution $u = \sqrt{1+c}$ shows that

$$N_{0,4}(a;m) = \frac{m\pi\sqrt{2}}{2^{6m+1}}\binom{4m}{2m}\binom{2m}{m}\int_1^\infty f_m(u)(a+u)^{-(2m+1/2)}\,\mathrm{d}u, \tag{8.39}$$

with $f_m(u) = u(u^2-1)^{m-1}$. This final integral can now be evaluated to give the desired expression (8.30) for $N_{0,4}$. To this end one integrates by parts and uses the fact that the derivatives of f_m at $u = 1$ have a closed-form evaluation. Further details can be found in [BM01].

8.6 Random walk integrals

In this section, the n-dimensional integral

$$W_n(s) := \int_{[0,1]^n}\left|\sum_{k=1}^n \mathrm{e}^{2\pi i x_k}\right|^s dx_1 dx_2\cdots dx_n \tag{8.40}$$

is considered which has recently been studied in [BNSW11] and [BSW11]. This integral is connected to planar random walks. In detail, such a walk is said to be *uniform* if it starts at the origin and at each step takes a unit-step in a random direction. As such, (8.40) expresses the s-th moment of the distance to the origin after n steps. The study of these walks originated with K. Pearson more than a century ago [Pea05a].

For s an even integer, the moments $W_n(s)$ take integer values. In fact, for integers $k \geqslant 0$, the explicit formula

$$W_n(2k) = \sum_{a_1+\cdots+a_n=k} \binom{k}{a_1, \ldots, a_n}^2 \tag{8.41}$$

has been established in [BNSW11]. The evaluation of $W_n(s)$ for values of $s \neq 2k$ is more challenging. In particular, the definition (8.40) is not well-suited for high-precision numerical evaluations, and other representations are needed.

In the remainder of this section, it is indicated how Ramanujan's Master Theorem may be applied to find a one-dimensional integral representation for $W_n(s)$. While (8.40) may be used to justify a priori that Ramanujan's Master Theorem 8.3.2 applies, it should be noted that one may proceed formally with only the sequence (8.41) given. This is the approach taken below in the proof of Theorem 8.6.1. Ramanujan's Master Theorem produces a formal candidate for an analytic extension of the sequence $W_n(2k)$. This argument yields the following Bessel integral representation of (8.40), previously obtained by D. Broadhurst [Bro09].

Theorem 8.6.1. *Let $s \in \mathbb{C}$ with $2k > \operatorname{Re} s > \max(-2, -\frac{n}{2})$. Then*

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1+\frac{s}{2})}{\Gamma(k-\frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x} \frac{\mathrm{d}}{\mathrm{d}x} \right)^k J_0^n(x) \, \mathrm{d}x. \tag{8.42}$$

Proof. The evaluation (8.41) yields the generating function for the even moments:

$$\sum_{k \geqslant 0} W_n(2k) \frac{(-x)^k}{(k!)^2} = \left(\sum_{k \geqslant 0} \frac{(-x)^k}{(k!)^2} \right)^n = J_0(2\sqrt{x})^n, \tag{8.43}$$

with $J_0(z)$ the Bessel function of the first kind as in (8.17). Applying Ramanujan's Master Theorem (8.1) to $\lambda(k) = W_n(2k)/k!$ produces

$$\Gamma(\nu)\lambda(-\nu) = \int_0^\infty x^{\nu-1} J_0^n(2\sqrt{x})\,\mathrm{d}x. \tag{8.44}$$

A change of variables and setting $s = 2\nu$ gives

$$W_n(-s) = 2^{1-s}\frac{\Gamma(1-s/2)}{\Gamma(s/2)}\int_0^\infty x^{s-1} J_0^n(x)\,\mathrm{d}x. \tag{8.45}$$

The claim now follows from the fact that if $F(s)$ is the Mellin transform of $f(x)$ then $(s-2)(s-4)\cdots(s-2k)F(s-2k)$ is the corresponding transform of $\left(-\frac{1}{x}\frac{\mathrm{d}}{\mathrm{d}x}\right)^k f(x)$. The latter is a consequence of Ramanujan's Master Theorem. □

8.7 Extending the domain of validity

The region of validity of the identity given by Ramanujan's Master Theorem is restricted by the region of convergence of the integral. For example, the integral representation of the gamma function given in (8.5) holds for Re $s > 0$. In this section it is shown that analytic continuations of such representations are readily available by dropping the first few terms of the Taylor series of the defining integrand. This provides an alternative to the method used at the end of the proof of Theorem 8.6.1.

Theorem 8.7.1. *Suppose φ satisfies the conditions of Theorem 8.3.2 so that for all* $0 < \mathrm{Re}\ s < \delta$

$$\int_0^\infty x^{s-1}\sum_{k=0}^\infty \varphi(k)(-x)^k\,\mathrm{d}x = \frac{\pi}{\sin s\pi}\varphi(-s).$$

Then, for any positive integer N and $-N < \mathrm{Re}\ s < -N+1$,

$$\int_0^\infty x^{s-1}\sum_{k=N}^\infty \varphi(k)(-x)^k\,\mathrm{d}x = \frac{\pi}{\sin s\pi}\varphi(-s). \tag{8.46}$$

Proof. Applying Theorem 8.3.2 to the function $\varphi(\cdot + N)$ shows that

$$\int_0^\infty x^{s-1} \sum_{k=0}^\infty \varphi(k+N)(-x)^k \, dx = \frac{\pi}{\sin s\pi} \varphi(-s+N).$$

Now shift s to obtain (8.46). □

Example 8.7.2. Apply the result (8.46) with $N = 1$ to obtain

$$\Gamma(s) = \int_0^\infty x^{s-1} \left(e^{-x} - 1 \right) \, dx. \tag{8.47}$$

This integral representation now gives an analytic continuation of (8.5) to $-1 < \text{Re } s < 0$.

8.8 Some classical polynomials

In this section the explicit formulas for the generating functions of classical polynomials are employed to derive some definite integrals.

8.8.1 The Bernoulli polynomials

The generating function for the Bernoulli polynomials $B_m(q)$ is given by

$$\frac{te^{qt}}{e^t - 1} = \sum_{m=0}^\infty B_m(q) \frac{t^m}{m!}. \tag{8.48}$$

These polynomials relate to the Hurwitz zeta function

$$\zeta(z, q) = \sum_{n=0}^\infty \frac{1}{(n+q)^z} \tag{8.49}$$

via $B_m(q) = -m\zeta(1-m,q)$ for $m \geq 1$. Then (8.48) yields

$$\frac{e^{-qt}}{1-e^{-t}} - \frac{1}{t} = \sum_{m=0}^{\infty} \zeta(-m,q)\frac{(-t)^m}{m!}. \tag{8.50}$$

Ramanujan's Master Theorem now provides the integral representation

$$\int_0^\infty t^{\nu-1}\left(\frac{e^{-qt}}{1-e^{-t}} - \frac{1}{t}\right) dt = \Gamma(\nu)\zeta(\nu,q), \tag{8.51}$$

valid in the range $0 < \text{Re}\ \nu < 1$.

8.8.2 The Hermite polynomials

The generating function for the Hermite polynomials $H_m(x)$ is

$$e^{2xt-t^2} = \sum_{m=0}^{\infty} H_m(x)\frac{t^m}{m!}. \tag{8.52}$$

Their analytic continuation, as a function in the index m, is given by

$$H_m(x) = 2^m U\left(-\frac{m}{2}, \frac{1}{2}, x^2\right) \tag{8.53}$$

where U is Whittaker's confluent hypergeometric function. Ramanujan's Master Theorem now provides the integral evaluation

$$\int_0^\infty t^{s-1}e^{-2xt-t^2}\, dt = \frac{\Gamma(s)}{2^s}\, U\left(\frac{s}{2}, \frac{1}{2}, x^2\right). \tag{8.54}$$

An equivalent form of this evaluation appears as Entry 3.462.1 in [GR80].

8.8.3 The Laguerre polynomials

The Laguerre polynomials $L_n(x)$ given by

$$\frac{1}{1-t}\exp\left(-\frac{xt}{1-t}\right) = \sum_{n=0}^{\infty} L_n(x)t^n \tag{8.55}$$

can be expressed also as $L_n(x) = M(-n, 1; x)$, where

$$M(a, c; x) = {}_1F_1\left(\begin{matrix} a \\ c \end{matrix}\middle| x\right) = \sum_{j=0}^{\infty} \frac{(a)_j}{(c)_j}\frac{x^j}{j!} \tag{8.56}$$

is the confluent hypergeometric or Kummer function. Ramanujan's Master Theorem yields the evaluation

$$\int_0^{\infty} \frac{t^{\nu-1}}{1+t}\exp\left(\frac{xt}{1+t}\right) \mathrm{d}t = \Gamma(\nu)\Gamma(1-\nu)M(\nu, 1; x). \tag{8.57}$$

The change of variables $r = t/(1+t)$ then gives

$$M(\nu, 1; x) = \frac{1}{\Gamma(\nu)\Gamma(1-\nu)} \int_0^1 r^{\nu-1}(1-r)^{-\nu}\mathrm{e}^{rx}\,\mathrm{d}r, \tag{8.58}$$

which is Entry 9.211.2 in [GR80].

8.8.4 The Jacobi polynomials

The Jacobi polynomials $P_n^{(\alpha,\beta)}(x)$ are defined by the generating function

$$\sum_{n=0}^{\infty} P_n^{(\alpha,\beta)}(x)t^n = \frac{2^{\alpha+\beta}}{R^*(x,t)}(1-t+R^*(x,t))^{-\alpha}(1+t+R^*(x,t))^{-\beta}, \tag{8.59}$$

where $R^*(x,t) = \sqrt{1-2xt+t^2}$. These polynomials admit the hypergeometric representation

$$P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(n+1+\alpha)}{n!\,\Gamma(1+\alpha)} {}_2F_1\left(n+\alpha+\beta+1, -n; 1+\alpha; \frac{1-x}{2}\right). \tag{8.60}$$

Now write $R(x,t) = R^*(x,-t)$, so that $R(x,t) = \sqrt{1+2xt+t^2}$, to obtain

$$2^{\alpha+\beta}R^{-1}(1+t+R)^{-\alpha}(1-t+R)^{-\beta} = \sum_{k=0}^{\infty} \lambda(k) \frac{(-t)^k}{k!} \tag{8.61}$$

where

$$\lambda(k) = \frac{\Gamma(k+1+\alpha)}{\Gamma(1+\alpha)} {}_2F_1\left(k+\alpha+\beta+1, -k; 1+\alpha; \frac{1-x}{2}\right). \tag{8.62}$$

Ramanujan's Master Theorem produces

$$\begin{aligned}\int_0^\infty & \frac{t^{\nu-1}\,\mathrm{d}t}{R(1+t+R)^{\alpha}(1-t+R)^{\beta}} \\ &= \frac{B(\nu, 1+\alpha-\nu)}{2^{\alpha+\beta}} {}_2F_1\left(\left. \begin{matrix} 1+\alpha+\beta-\nu, \nu \\ 1+\alpha \end{matrix} \right| \frac{1-x}{2} \right).\end{aligned}$$

8.8.5 The Chebyshev polynomials of the second kind

These polynomials are defined by

$$U_n(a) = \frac{\sin((n+1)x)}{\sin x}, \quad \text{where } \cos x = a, \tag{8.63}$$

and have the generating function

$$\sum_{k=0}^{\infty} U_k(a)x^k = \frac{1}{1-2ax+x^2}. \tag{8.64}$$

The usual application of Ramanujan's Master Theorem yields

$$\int_0^\infty \frac{x^{\nu-1}\,\mathrm{d}x}{1+2ax+x^2} = \frac{\pi}{\sin \pi\nu}\,\frac{\sin[(1-\nu)\cos^{-1} a]}{\sqrt{1-a^2}}. \tag{8.65}$$

This result appears as Entry 3.252.12 in [GR80].

8.9 The method of brackets

The focus of this final section will be on a multi-dimensional extension of Ramanujan's Master Theorem. This has been called the *method of brackets* and it was originally presented in [GS07] in the context of integrals arising from Feynman diagrams. A complete description of the operational rules of the method, together with a variety of examples, was first discussed in [GM10]. The basic idea is the assignment of a formal symbol $\langle a \rangle$ to the divergent integral

$$\int_0^\infty x^{a-1}\,\mathrm{d}x. \tag{8.66}$$

The rules for operating with brackets are described below. These rules employ the symbol

$$\phi_n = \frac{(-1)^n}{\Gamma(n+1)}, \tag{8.67}$$

called the *indicator of* n.

Rule 8.9.1. *The bracket expansion*

$$\frac{1}{(a_1+a_2+\cdots+a_r)^\alpha} = \sum_{m_1,\ldots,m_r} \phi_{m_1,\ldots,m_r} a_1^{m_1}\cdots a_r^{m_r}\,\frac{\langle \alpha+m_1+\cdots+m_r\rangle}{\Gamma(\alpha)}$$

holds. Here $\phi_{m_1,\ldots,m_r}$ is a shorthand notation for the product $\phi_{m_1}\cdots\phi_{m_r}$. Where there is no possibility of confusion this will be further abridged as $\phi_{\{m\}}$. The notation $\sum_{\{m\}}$ is to be understood likewise.

Rule 8.9.2. *A series of brackets*

$$\sum_{\{n\}} \phi_{\{n\}} f(n_1,\ldots,n_r)\, \langle a_{11}n_1 + \cdots a_{1r}n_r + c_1\rangle \cdots \langle a_{r1}n_1 + \cdots a_{rr}n_r + c_r\rangle$$

is assigned the value

$$\frac{1}{|det(A)|} f(n_1^*,\cdots,n_r^*)\Gamma(-n_1^*)\cdots\Gamma(-n_r^*),$$

where A is the matrix of coefficients (a_{ij}) and (n_i^*) is the solution of the linear system obtained by the vanishing of the brackets. No value is assigned if the matrix A is singular.

Rule 8.9.3. *In the case where a higher dimensional series has more summation indices than brackets, the appropriate number of free variables is chosen among the indices. For each such choice, Rule 8.9.2 yields a series. Those converging in a common region are added to evaluate the desired integral.*

Example 8.9.4. Apply the method of brackets to

$$\int_0^\infty x^{\nu-1} F(x)\, \mathrm{d}x \tag{8.68}$$

where F has the series representation

$$F(x) = \sum_{k=0}^\infty \phi_k \lambda(k) x^k.$$

Then (8.68) can be written as the bracket series

$$\int_0^\infty x^{\nu-1}F(x)\,\mathrm{d}x = \int_0^\infty \sum_{k=0}^\infty \phi_k \lambda(k) x^{k+\nu-1}\,\mathrm{d}x = \sum_k \phi_k \lambda(k)\left\langle k+\nu\right\rangle.$$

Rule 8.9.2 assigns the value

$$\sum_k \phi_k \lambda(k)\left\langle k+\nu\right\rangle = \lambda(k^*)\Gamma(-k^*) \tag{8.69}$$

where k^* is the solution of $k+\nu=0$. Thus one obtains

$$\int_0^\infty x^{\nu-1}F(x)\,\mathrm{d}x = \lambda(-\nu)\Gamma(\nu). \tag{8.70}$$

This is precisely Ramanujan's Master Theorem as given by Theorem 8.3.2.

Rule 8.9.1 is a restatement of the fact that the Mellin transform of e^{-x} is $\Gamma(s)$:

$$\begin{aligned}\frac{\Gamma(s)}{(a_1+\ldots+a_r)^s} &= \int_0^\infty x^{s-1}\mathrm{e}^{-(a_1+\ldots+a_r)x}\,\mathrm{d}x \\ &= \int_0^\infty x^{s-1}\prod_{i=1}^r \sum_{m_i} \phi_{m_i}(a_i x)^{m_i}\,\mathrm{d}x \\ &= \sum_{\{m\}} \phi_{\{m\}} a_1^{m_1}\cdots a_r^{m_r}\left\langle s+m_1+\cdots+m_r\right\rangle.\end{aligned}$$

Example 8.9.4 has shown that the 1-dimensional version of Rule 8.9.2 is Ramanujan's Master Theorem. A formal argument is now presented to show that the multi-dimensional version of Rule 8.9.2 follows upon iterating the one-dimensional result. The exposition is restricted to the 2-dimensional case. Consider the bracket series

$$\sum_{n_1,n_2} \phi_{n_1}\phi_{n_2} f(n_1,n_2)\left\langle a_{11}n_1+a_{12}n_2+c_1\right\rangle\left\langle a_{21}n_1+a_{22}n_2+c_2\right\rangle \tag{8.71}$$

which encodes the integral

$$\int_0^\infty \int_0^\infty \sum_{n_1,n_2} \phi_{n_1}\phi_{n_2} f(n_1,n_2) x^{a_{11}n_1+a_{12}n_2+c_1-1} y^{a_{21}n_1+a_{22}n_2+c_2-1}\, \mathrm{d}x\, \mathrm{d}y.$$

Substituting $(u,v) = (x^{a_{11}}y^{a_{21}}, x^{a_{12}}y^{a_{22}})$ yields $\frac{\mathrm{d}x\mathrm{d}y}{xy} = \frac{1}{|a_{11}a_{22}-a_{12}a_{21}|}\frac{\mathrm{d}u\mathrm{d}v}{uv}$, and hence the above integral simplifies to

$$\frac{1}{|a_{11}a_{22}-a_{12}a_{21}|}\int_0^\infty \int_0^\infty \sum_{n_1,n_2} \phi_{n_1}\phi_{n_2} f(n_1,n_2) u^{n_1-n_1^*-1} v^{n_2-n_2^*-1}\, \mathrm{d}u\, \mathrm{d}v.$$

Here (n_1^*, n_2^*) is the solution to $a_{11}n_1^* + a_{12}n_2^* + c_1 = 0$, $a_{21}n_1^* + a_{22}n_2^* + c_2 = 0$. Ramanujan's Master Theorem gives

$$\int_0^\infty \sum_{n_1} \phi_{n_1} f(n_1,n_2) u^{n_1-n_1^*-1}\, \mathrm{d}u = f(n_1^*, n_2)\Gamma(-n_1^*).$$

A second application of Ramanujan's Master Theorem shows that the bracket series (8.71) evaluates to

$$\frac{1}{|a_{11}a_{22}-a_{12}a_{21}|} f(n_1^*, n_2^*)\Gamma(-n_1^*)\Gamma(-n_2^*).$$

This is Rule 8.9.2.

8.9.1 A gamma-like higher dimensional integral

The next example illustrates the power and ease of the method of brackets for the treatment of certain multidimensional integrals such as

$$\int_0^\infty \cdots \int_0^\infty \exp\left(-(x_1+\ldots+x_n)^\alpha\right) \prod_{i=1}^n x_i^{s_i-1}\, \mathrm{d}x_i. \tag{8.72}$$

It should be pointed out that this class of integrals is beyond the scope of current computer algebra systems including `Mathematica` 7 and `Maple` 12.

For simplicity of exposition, take $n = 2$ in (8.72). The n-dimensional case presents no additional difficulties.

$$\begin{aligned}
&\int_0^\infty \int_0^\infty x^{s-1} y^{t-1} \exp\left(-(x+y)^\alpha\right) \, \mathrm{d}x \, \mathrm{d}y \\
&= \sum_j \phi_j \int_0^\infty \int_0^\infty x^{s-1} y^{t-1} (x+y)^{\alpha j} \, \mathrm{d}x \, \mathrm{d}y \\
&= \sum_j \phi_j \int_0^\infty \int_0^\infty x^{s-1} y^{t-1} \sum_{n,m} \phi_{n,m} x^n y^m \frac{\langle n+m-\alpha j\rangle}{\Gamma(-\alpha j)} \, \mathrm{d}x \, \mathrm{d}y \\
&= \sum_{j,n,m} \phi_{j,n,m} \frac{1}{\Gamma(-\alpha j)} \langle n+m-\alpha j\rangle \langle n+s\rangle \langle m+t\rangle
\end{aligned}$$

Solving the linear equations for the vanishing of the brackets gives $n^* = -s$, $m^* = -t$, and $j^* = -\frac{s+t}{\alpha}$. The determinant of the system is α, therefore the integral is

$$\frac{1}{\alpha} \frac{1}{\Gamma(-\alpha j^*)} \Gamma(-n^*)\Gamma(-m^*)\Gamma(-j^*) = \frac{1}{\alpha} \frac{\Gamma(s)\Gamma(t)}{\Gamma(s+t)} \Gamma\left(\frac{s+t}{\alpha}\right).$$

The full statement of this result is presented as the next theorem.

Theorem 8.9.5.

$$\begin{aligned}
&\int_0^\infty \cdots \int_0^\infty \exp\left(-(x_1 + \ldots + x_n)^\alpha\right) \prod_{i=1}^n x_i^{s_i - 1} \, \mathrm{d}x_i \\
&\quad = \frac{1}{\alpha} \frac{\Gamma(s_1)\Gamma(s_2)\ldots\Gamma(s_n)}{\Gamma(s_1 + \ldots + s_n)} \Gamma\left(\frac{s_1 + \ldots + s_n}{\alpha}\right).
\end{aligned}$$

Remark 8.9.6. The correct interpretation of Rule 8.9.3 is work in-progress. The next example illustrates the subtleties associated with this question. The evaluation

$$\int_0^\infty x^{s-1} \mathrm{e}^{-2x} \, \mathrm{d}x = \frac{\Gamma(s)}{2^s} \tag{8.73}$$

follows directly from the bracket expansion

$$\int_0^\infty x^{s-1} \mathrm{e}^{-2x} \, \mathrm{d}x = \sum_n \phi_n 2^n \langle n+s \rangle$$

and Rule 8.9.2. On the other hand, rewriting the integrand as $\mathrm{e}^{-2x} = \mathrm{e}^{-x}\mathrm{e}^{-x}$ and expanding it in a bracket series produces

$$\int_0^\infty x^{s-1} \mathrm{e}^{-x}\mathrm{e}^{-x} \, \mathrm{d}x = \sum_{n,m} \phi_{n,m} \langle n+m+s \rangle .$$

The resulting bracket series has more summation indices than brackets. The choice of n as a free variable, gives $m^* = -n-s$ and Rule 8.9.2 produces the convergent series

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \Gamma(n+s) = \Gamma(s) {}_1F_0 \left(\left. \begin{matrix} s \\ - \end{matrix} \right| -1 \right) = \frac{\Gamma(s)}{2^s}. \tag{8.74}$$

Symmetry dictates that the choice of m as a free variable leads to the same result. Rule 8.9.3, as stated currently, would yield the correct evaluation (8.73), twice.

The trouble has its origin in that the series in (8.74) has been evaluated at the boundary of its region of convergence. Rule 8.9.3 should be modified by introducing extra parameters to distinguish different regions of convergence. This remains to be clarified. For instance,

$$\int_0^\infty x^{s-1} \mathrm{e}^{-Ax}\mathrm{e}^{-Bx} \, \mathrm{d}x = \sum_{n,m} \phi_{n,m} A^n B^m \langle n+m+s \rangle \tag{8.75}$$

which, upon choosing n and m as free variables, yields the two series

$$\frac{\Gamma(s)}{B^s} {}_1F_0 \left(\left. \begin{matrix} s \\ - \end{matrix} \right| -\frac{A}{B} \right), \qquad \frac{\Gamma(s)}{A^s} {}_1F_0 \left(\left. \begin{matrix} s \\ - \end{matrix} \right| -\frac{B}{A} \right)$$

respectively. Both series evaluate to $\Gamma(s)/(A+B)^s$, but it is now apparent that their regions of convergence are different. Accordingly, they should not be added in order to obtain the value (8.75). The original integral (8.73) appears as the limit $A, B \to 1$.

Chapter 9

The method of brackets. Part 2: Examples and applications

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

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(with Ivan Gonzalez, Victor H. Moll)
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Abstract A new heuristic method for the evaluation of definite integrals is presented. This *method of brackets* has its origin in methods developed for the evaluation of Feynman diagrams. The operational rules are described and the method is illustrated with several examples. The method of brackets reduces the evaluation of a large class of definite integrals to the solution of a linear system of equations.

9.1 Introduction

The *method of brackets* presented here provides a method for the evaluation of a large class of definite integrals. The ideas were originally presented in [GS07] in the context of integrals arising from Feynman diagrams. A complete description of the operational rules of the method together with a variety of examples was first discussed in [GM10].

The method is quite simple to work with and many of the entries from the classical table of integrals [GR80] can be derived using this method. The basic idea is to introduce the formal symbol $\langle a \rangle$, called a *bracket*, which represents the divergent integral

$$\int_0^\infty x^{a-1}\,\mathrm{d}x. \tag{9.1}$$

The formal rules for operating with these brackets are described in Section 9.2 and their justification (especially of the heuristic Rule 9.2.5) is work-in-progress. In particular, convergence issues are ignored at the moment. Roughly, each integral generates a linear system of equations and for each choice of free variables the method yields a series with the free variables as summation indices. A heuristic rule states that those converging in a common region give the desired evaluation.

Section 9.3 illustrates the method by evaluating the Laplace transform of the Bessel function $J_\nu(x)$. In this example, the two resulting series converge in different regions and are analytic continuations of each other. This is a general phenomenon which is used in Section 9.5 to produce an explicit analytic continuation of the hypergeometric function ${}_{q+1}F_q(x)$. Section 9.4 presents the evaluation of a family of integrals C_n appearing in Statistical Mechanics. These were introduced in [BBC06] as a toy model and their physical interpretation was discovered later. The method of brackets is employed here to evaluate the first four values, the only known cases (an expression for the next value C_5 in terms of a double hypergeometric series is possible but is not given here). The last section employs the method of brackets to resolve a Feynman diagram.

9.2 The method of brackets

The method of brackets discussed in this paper is based on the assignment of the formal symbol $\langle a \rangle$ to the divergent integral (9.1).

Example 9.2.1. If f is given by the formal power series

$$f(x) = \sum_{n=0}^{\infty} a_n x^{\alpha n + \beta - 1},$$

then the improper integral of f over the positive real axis is formally written as the *bracket series*

$$\int_0^{\infty} f(x)\,\mathrm{d}x = \sum_n a_n \langle \alpha n + \beta \rangle . \tag{9.2}$$

Here, and in the sequel, $\sum_n$ is used as a shorthand for $\sum_{n=0}^{\infty}$.

Formal rules for operating with brackets are described next. In particular, Rule 9.2.4 describes how to evaluate a bracket series such as the one appearing in (9.2). To this end, it is useful to introduce the symbol

$$\phi_n = \frac{(-1)^n}{\Gamma(n+1)}, \tag{9.3}$$

which is called the *indicator of* n.

Example 9.2.2. The gamma function has the bracket expansion

$$\Gamma(a) = \int_0^{\infty} x^{a-1} e^{-x}\,\mathrm{d}x = \sum_n \phi_n \langle n + a \rangle . \tag{9.4}$$

Rule 9.2.3. *The bracket expansion*

$$\frac{1}{(a_1 + a_2 + \cdots + a_r)^{\alpha}} = \sum_{m_1,\ldots,m_r} \phi_{m_1,\ldots,m_r} a_1^{m_1} \cdots a_r^{m_r} \frac{\langle \alpha + m_1 + \cdots + m_r \rangle}{\Gamma(\alpha)} \tag{9.5}$$

holds. Here $\phi_{m_1,\ldots,m_r}$ is a shorthand notation for the product $\phi_{m_1}\cdots\phi_{m_r}$. If there is no possibility of confusion this will be further abridged as $\phi_{\{m\}}$. The notation $\sum_{\{m\}}$ is to be understood likewise.

Rule 9.2.4. *A series of brackets is assigned a value according to*

$$\sum_{n} \phi_n f(n) \langle an+b \rangle = \frac{1}{|a|} f(n^*)\Gamma(-n^*), \tag{9.6}$$

where n^* is the solution of the equation $an+b=0$. Observe that this might result in the replacing of the index n, initially a nonnegative integer, by a complex number n^*.

Similarly, a higher dimensional bracket series, that is,

$$\sum_{\{n\}} \phi_{\{n\}} f(n_1,\ldots,n_r) \langle a_{11}n_1 + \cdots a_{1r}n_r + c_1 \rangle \cdots \langle a_{r1}n_1 + \cdots a_{rr}n_r + c_r \rangle$$

is assigned the value

$$\frac{1}{|det(A)|} f(n_1^*,\cdots,n_r^*)\Gamma(-n_1^*)\cdots\Gamma(-n_r^*), \tag{9.7}$$

where A is the matrix of coefficients (a_{ij}) and (n_i^*) is the solution of the linear system obtained by the vanishing of the brackets. The value is not defined if the matrix A is not invertible.

Rule 9.2.5. *In the case where a higher dimensional series has more summation indices than brackets, the appropriate number of free variables is chosen among the indices. For each such choice, Rule 9.2.4 yields a series. Those converging in a common region are added to evaluate the desired integral.*

9.3 An example from Gradshteyn and Ryzhik

The second author is involved in a long term project of providing proofs of all the entries from the classical table of integrals by Gradshteyn and Ryzhik [GR80]. The proofs can be found at:

http://www.math.tulane.edu/~vhm/Table.html

In this section the method of brackets is illustrated to find

$$\int_0^\infty x^\nu e^{-\alpha x} J_\nu(\beta x)\, \mathrm{d}x = \frac{(2\beta)^\nu \Gamma(\nu + \frac{1}{2})}{\sqrt{\pi}(\alpha^2 + \beta^2)^{\nu+1/2}} \tag{9.8}$$

which is entry 6.623.1 of [GR80]. Here

$$J_\nu(x) = \sum_{k=0}^\infty \frac{(-1)^k (x/2)^{2k+\nu}}{k!\, \Gamma(k+\nu+1)} \tag{9.9}$$

is the Bessel function of order ν. To this end, the integrand is expanded as

$$\begin{aligned} e^{-\alpha x} J_\nu(\beta x) &= \left(\sum_n \phi_n (\alpha x)^n \right) \left(\sum_k \phi_k \frac{(\frac{\beta x}{2})^{2k+\nu}}{\Gamma(k+\nu+1)} \right) \\ &= \sum_{k,n} \phi_{k,n} \frac{\alpha^n (\frac{\beta}{2})^{2k+\nu}}{\Gamma(k+\nu+1)} x^{n+2k+2\nu}, \end{aligned} \tag{9.10}$$

so as to obtain the bracket series

$$\int_0^\infty e^{-\alpha x} J_\nu(\beta x) \mathrm{d}x = \sum_{k,n} \phi_{k,n} \frac{\alpha^n (\frac{\beta}{2})^{2k+\nu}}{\Gamma(k+\nu+1)} \langle n + 2k + 2\nu + 1 \rangle . \tag{9.11}$$

The evaluation of this double sum by the method of brackets produces two series corresponding to using either k or n as the free variable when applying Rule 9.2.4.

The index k is free

Choosing k as the free variable when applying Rule 9.2.4 to (9.11), yields $n^* = -2k - 2\nu - 1$ and thus the resulting series

$$\begin{aligned} &\sum_k \phi_k \frac{\alpha^{-2k-2\nu-1}(\frac{\beta}{2})^{2k+\nu}}{\Gamma(k+\nu+1)}\Gamma(2k+2\nu+1) \\ &= \alpha^{-2\nu-1}(\tfrac{\beta}{2})^{\nu}\frac{\Gamma(2\nu+1)}{\Gamma(\nu+1)}\,{}_1F_0\left(\begin{matrix}\nu+\frac{1}{2}\\ -\end{matrix}\middle| -\frac{\beta^2}{\alpha^2}\right). \end{aligned} \tag{9.12}$$

The right-hand side employs the usual notation for the hypergeometric function

$${}_pF_q\left(\begin{matrix}a_1,\ldots,a_p\\ b_1,\ldots,b_q\end{matrix}\middle| x\right) = \sum_{n=0}^{\infty}\frac{(a_1)_n\cdots(a_p)_n}{(b_1)_n\cdots(b_q)_n}\frac{x^n}{n!} \tag{9.13}$$

where $(\alpha)_n = \frac{\Gamma(\alpha+n)}{\Gamma(\alpha)}$ is the Pochhammer symbol. Note that the ${}_1F_0$ in (9.12) converges provided $|\beta| < |\alpha|$. In this case, the standard identity ${}_1F_0(a|x) = (1-x)^{-a}$ together with the duplication formula for the Γ function shows that the series in (9.12) is indeed equal to the right-hand side of (9.8).

The index n is free

In this second case, the linear system in Rule 9.2.4 has determinant 2 and yields $k^* = -n/2 - \nu - 1/2$. This gives

$$\frac{1}{2}\sum_n \phi_n \frac{\alpha^n(\frac{\beta}{2})^{-n-\nu-1}}{\Gamma(-n/2+1/2)}\Gamma(n/2+\nu+1/2). \tag{9.14}$$

This series now converges provided that $|\beta| > |\alpha|$ in which case it again sums to the right-hand side of (9.8).

Note 9.3.1. This is the typical behavior of the method of brackets. The different choices of indices as free variables give representations of the solution valid in different regions. Each of these is an analytic continuation of the other ones.

9.4 Integrals of the Ising class

In this section the method of brackets is used to discuss the integral

$$C_n = \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n}. \tag{9.15}$$

This family was introduced in [BBC06] as a caricature of the *Ising susceptibility integrals*

$$D_n = \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \prod_{i<j} \left(\frac{u_i - u_j}{u_i + u_j}\right)^2 \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n}. \tag{9.16}$$

Actually, the integrals C_n appear naturally in the analysis of certain amplitude transforms [PT81]. The first few values are given by

$$C_1 = 2,\ C_2 = 1,\ C_3 = L_{-3}(2),\ C_4 = \frac{7}{12}\zeta(3). \tag{9.17}$$

Here, L_D is the Dirichlet L-function. In this case,

$$L_{-3}(2) = \sum_{n=0}^\infty \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2}\right). \tag{9.18}$$

No analytic expression for C_n is known for $n \geqslant 5$. Similarly,

$$D_1 = 2,\ D_2 = \frac{1}{3},\ D_3 = 8 + \frac{4\pi^2}{3} - 27L_{-3}(2),\ D_4 = \frac{4\pi^2}{9} - \frac{1}{6} - \frac{7}{12}\zeta(3) \tag{9.19}$$

are given in [BBC06]. High precision numerical evaluation and PSLQ experiments have further produced the conjecture

$$D_5 = 42 - 1984\,\mathrm{Li}_4(\tfrac{1}{2}) + \frac{189}{10}\pi^4 - 74\zeta(3) - 1272\zeta(3)\ln 2 + 40\pi^2\ln^2 2 \\ - \frac{62}{3}\pi^3 + \frac{40}{3}\pi^2\ln 2 + 88\ln^4 2 + 464\ln^2 2 - 40\ln 2. \tag{9.20}$$

The integral C_n is the special case $k = 1$ of the family

$$C_{n,k} = \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^{k+1}} \frac{\mathrm{d}u_1}{u_1} \cdots \frac{\mathrm{d}u_n}{u_n} \tag{9.21}$$

that also gives the moments of powers of the Bessel function K_0 via

$$C_{n,k} = \frac{2^{n-k+1}}{n!\,k!} c_{n,k} := \frac{2^{n-k+1}}{n!\,k!} \int_0^\infty t^k K_0^n(t)\,\mathrm{d}t. \tag{9.22}$$

The values

$$c_{1,k} = 2^{k-1}\Gamma^2\left(\frac{k+1}{2}\right), \quad c_{2,k} = \frac{\sqrt{\pi}}{4}\frac{\Gamma^3\left(\frac{k+1}{2}\right)}{\Gamma\left(\frac{k}{2}+1\right)}, \tag{9.23}$$

as well as the recursion

$$(k+1)^4 c_{3,k} - 2(5k^2 + 20k + 21)c_{3,k+2} + 9c_{3,k+4} = 0 \tag{9.24}$$

with initial data

$$c_{3,0} = \frac{3\alpha}{32\pi},\ c_{3,1} = \frac{3}{4}L_{-3}(2),\ c_{3,2} = \frac{\alpha}{96\pi} - \frac{4\pi^5}{9\alpha},\ c_{3,3} = L_{-3}(2) - \frac{2}{3}, \tag{9.25}$$

where $\alpha = 2^{-2/3}\Gamma^6(\frac{1}{3})$ are given in [BBBG08] and [BS08].

The evaluation of these integrals presented in the literature usually begins with the introduction of spherical coordinates. This reduces the dimension of C_n by two and immediately gives the values of C_1 and C_2. The evaluation of C_3 is reduced to the logarithmic integral

$$C_3 = \frac{2}{3}\int_0^\infty \frac{\ln(1+x)\,\mathrm{d}x}{x^2+x+1}. \tag{9.26}$$

Its value is obtained by the change of variables $x \to \frac{1}{t} - 1$ followed by an expansion of the integrand. A systematic discussion of these type of logarithmic integrals is provided in [MM09]. The value of C_4 is obtained via the double integral representation

$$C_4 = \frac{1}{6}\int_0^\infty \int_0^\infty \frac{\ln(1+x+y)}{(1+x+y)(1+1/x+1/y)-1}\frac{\mathrm{d}x}{x}\frac{\mathrm{d}y}{y}. \tag{9.27}$$

Moreover, the limiting behavior

$$\lim_{n\to\infty} C_n = 2e^{-2\gamma} \tag{9.28}$$

was established in [BBC06].

In this section the method of brackets is used to obtain the expressions for C_2, C_3, and C_4 described above. An advantage of this method is that it systematically gives an analytic expression for these integrals. When applied to C_5, the method produces a double series representation which is not discussed here.

9.4.1 Evaluation of $C_{2,k}$

The numbers $C_{2,k}$ are given by

$$C_{2,k} = 2\int_0^\infty \int_0^\infty \frac{\mathrm{d}x\,\mathrm{d}y}{xy\,\left(x+1/x+y+1/y\right)^{k+1}}. \tag{9.29}$$

A direct application of the method of brackets, by applying Rule 9.2.3 to the integrand as in (9.29), results in a bracket expansion involving a 4-fold sum and 3 brackets. Rules 9.2.4 and 9.2.5 translates this into a collection of series with $4-3=1$ summation indices. However, it is generally desirable to minimize the final number of summations by reducing the number of sums and increasing the number of brackets. In this example this is achieved by writing

$$\begin{aligned} C_{2,k} &= 2\int_0^\infty \int_0^\infty \frac{(xy)^k \,\mathrm{d}x\,\mathrm{d}y}{(x^2y+y+xy^2+x)^{k+1}} \\ &= 2\int_0^\infty \int_0^\infty \frac{(xy)^k \,\mathrm{d}x\,\mathrm{d}y}{(xy\,[x+y]+[x+y])^{k+1}}. \end{aligned}$$

In the evaluation of these expressions, the term $(x+y)$ must be expanded at the last step. The method of brackets now yields

$$\frac{1}{(xy\,[x+y]+[x+y])^{k+1}} = \sum_{n_1,n_2} \phi_{n_1,n_2}\; x^{n_1} y^{n_1}\,(x+y)^{n_1+n_2}\,\frac{\langle k+1+n_1+n_2\rangle}{\Gamma(k+1)},$$

and the expansion of the term $(x+y)$ gives

$$\frac{1}{(x+y)^{-n_1-n_2}} = \sum_{n_3,n_4} \phi_{n_3,n_4}\; x^{n_3} y^{n_4}\,\frac{\langle -n_1-n_2+n_3+n_4\rangle}{\Gamma(-n_1-n_2)}.$$

Replacing in the integral produces the bracket expansion

$$\begin{aligned} C_{2,k} = 2\sum_{\{n\}} \phi_{\{n\}} &\frac{\langle k+1+n_1+n_2\rangle}{\Gamma(k+1)}\frac{\langle -n_1-n_2+n_3+n_4\rangle}{\Gamma(-n_1-n_2)} \\ &\times \langle k+1+n_1+n_3\rangle\,\langle k+1+n_1+n_4\rangle\,. \end{aligned}$$

The value of this formal sum is now obtained by solving the linear system $k+1+n_1+n_2=0$, $-n_1-n_2+n_3+n_4=0$, $k+1+n_1+n_3=0$, and $k+1+n_1+n_4=0$ coming from the vanishing of brackets. This system has determinant 2 and its unique solution is $n_1^*=n_2^*=n_3^*=n_4^*=-\frac{k+1}{2}$. It follows that

$$C_{2,k} = \frac{\Gamma(-n_1^*)\,\Gamma(-n_2^*)\,\Gamma(-n_3^*)\,\Gamma(-n_4^*)}{\Gamma(k+1)\Gamma(-n_1^*-n_2^*)} = \frac{\Gamma\left(\frac{k+1}{2}\right)^4}{\Gamma(k+1)^2}. \tag{9.30}$$

Note that, upon employing Legendre's duplication formula for the Γ function, this evaluation is equivalent to (9.23). In particular, this confirms the value $C_2 = C_{2,1} = 1$ in (9.17).

Remark 9.4.1. The evaluation

$$\begin{aligned} C_{2,k}(\alpha,\beta) &= 2\int_0^\infty \int_0^\infty \frac{x^{\alpha-1}y^{\beta-1}\,\mathrm{d}x\,\mathrm{d}y}{(x+1/x+y+1/y)^{k+1}} \\ &= \frac{\Gamma\left(\frac{k+1+\alpha+\beta}{2}\right)\Gamma\left(\frac{k+1-\alpha-\beta}{2}\right)\Gamma\left(\frac{k+1+\alpha-\beta}{2}\right)\Gamma\left(\frac{k+1-\alpha+\beta}{2}\right)}{\Gamma(k+1)^2} \end{aligned} \tag{9.31}$$

that generalizes $C_{2,k}$ is obtained as a bonus. Similarly,

$$\begin{aligned} J_{r,s}(\alpha,\beta) &= 2\int_0^\infty \int_0^\infty \frac{x^{\alpha-1}y^{\beta-1}\,\mathrm{d}x\,\mathrm{d}y}{(x+y)^r(xy+1)^s} \\ &= \frac{\Gamma\left(\frac{-r+\alpha+\beta}{2}\right)\Gamma\left(\frac{2s+r-\alpha-\beta}{2}\right)\Gamma\left(\frac{r+\alpha-\beta}{2}\right)\Gamma\left(\frac{r-\alpha+\beta}{2}\right)}{\Gamma(r)\Gamma(s)}. \end{aligned} \tag{9.32}$$

Note that $C_{2,k}(\alpha,\beta) = J_{k+1,k+1}(\alpha+k+1,\beta+k+1)$.

Remark 9.4.2. The Ising susceptibility integral D_2, see (9.16), is obtained directly from the expression for $J_{r,s}$ given above. Indeed,

$$\begin{aligned} D_2 &= 2\int_0^\infty \int_0^\infty (x^2-2xy+y^2)\frac{xy\,\mathrm{d}x\,\mathrm{d}y}{(x+y)^4(xy+1)^2} \\ &= 2\left(J_{4,2}(4,2) - 2J_{4,2}(3,3) + J_{4,2}(2,4)\right) \\ &= \frac{1}{3}. \end{aligned} \tag{9.33}$$

This agrees with (9.19). This technique also yields the generalization

$$\begin{aligned} D_2(\alpha,\beta) &= 2\int_0^\infty \int_0^\infty \left(\frac{x-y}{x+y}\right)^2 \frac{x^{\alpha-1}y^{\beta-1}\,\mathrm{d}x\,\mathrm{d}y}{(x+1/x+y+1/y)^2} \\ &= \frac{(b-a)(b+a)(2+(b-a)^2)\pi^2}{12(\cos(\alpha\pi)-\cos(\beta\pi))} \end{aligned} \tag{9.34}$$

with limiting case $D_2(\alpha,\alpha) = \frac{1}{3}\frac{\alpha\pi}{\sin(\alpha\pi)}$.

9.4.2 Evaluation of $C_{3,k}$

Next, consider the integral

$$\begin{aligned} C_{3,k} &= \frac{2}{3}\int_0^\infty \int_0^\infty \int_0^\infty \frac{\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{xyz\,\left(x+1/x+y+1/y+z+1/z\right)^{k+1}} \\ &= \frac{2}{3}\int_0^\infty \int_0^\infty \int_0^\infty \frac{(xyz)^k\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{\left(xyz\,(x+y)+z\,(x+y)+xyz^2+xy\right)^{k+1}}. \end{aligned} \tag{9.35}$$

The second form of the integrand is motivated by the desire to to minimize the number of sums and to maximize the number of brackets in the expansion. The denominator is now expanded as

$$\sum_{\{n\}} \phi_{\{n\}} (xy)^{n_1+n_3+n_4} z^{n_1+n_2+2n_3}\,(x+y)^{n_1+n_2}\,\frac{\langle k+1+n_1+n_2+n_3+n_4\rangle}{\Gamma\,(k+1)},$$

and further expanding $(x+y)^{n_1+n_2}$ as

$$(x+y)^{n_1+n_2} = \sum_{n_5,n_6} \phi_{n_5,n_6}\; x^{n_5} y^{n_6} \frac{\langle -n_1-n_2+n_5+n_6\rangle}{\Gamma(-n_1-n_2)}$$

produces a complete bracket expansion of the integrand of $C_{3,k}$. Integration then yields

$$\begin{aligned} C_{3,k} = \frac{2}{3}\frac{1}{k!} \sum_{\{n\}} \phi_{\{n\}}\; & \frac{\langle -n_1-n_2+n_5+n_6\rangle}{\Gamma\,(-n_1-n_2)} \\ & \times \langle k+1+n_1+n_2+n_3+n_4\rangle\,\langle k+1+n_1+n_3+n_4+n_5\rangle \\ & \times \langle k+1+n_1+n_3+n_4+n_6\rangle\,\langle k+1+n_1+n_2+2n_3\rangle\,. \end{aligned} \tag{9.36}$$

This expression is regularized by replacing the bracket $\langle k+1+n_1+n_2+2n_3\rangle$ with $\langle k+1+n_1+n_2+2n_3+\epsilon\rangle$ with the intent of letting $\epsilon \to 0$. (This corresponds to multiplying the initial integrand with z^ϵ; however, note that many other regularizations are possible and eventually lead to Theorem 9.4.3. It will become clear shortly, see (9.38), why regularizing is necessary.) The method of brackets now gives a set of series expansions obtained by the vanishing of the five brackets in (9.36). The solution of the corresponding linear system (which has determinant 2) leaves one free index and produces the integral as a series in this variable. Of the six possible free indices, only n_3 and n_4 produce convergent series (more specifically, for each free index one obtains a hypergeometric series ${}_3F_2$ times an expression free of the index; for the indices n_3, n_4 the argument of this ${}_3F_2$ is $\frac{1}{4}$ while otherwise it is 4.) The heuristic Rule 9.2.5 states that their sum yields the value of the integral:

$$C_{3,k} = \frac{1}{3}\lim_{\epsilon\to 0}\frac{1}{k!}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}(f_{k,n}(\epsilon)+f_{k,n}(-\epsilon)) \tag{9.37}$$

where

$$f_{k,n}(\epsilon) = \frac{\Gamma\left(n+\frac{k+1+\epsilon}{2}\right)^4\Gamma(-n-\epsilon)}{\Gamma(2n+k+1+\epsilon)}. \tag{9.38}$$

Observe that the terms $f_{k,n}(\epsilon)$ are contributed by the index n_3 while the terms $f_{k,n}(-\epsilon)$ come from the index n_4. At $\epsilon = 0$, each of them has a simple pole. Consequently, the even combination $f_{k,n}(\epsilon)+f_{k,n}(-\epsilon)$ has no pole at $\epsilon = 0$. Using the expansions

$$\Gamma(x+\epsilon) = \Gamma(x)(1+\psi(x)\epsilon)+O(\epsilon^2), \tag{9.39}$$

for $x \neq 0, -1, -2, \ldots$, as well as

$$\Gamma(-n+\epsilon) = \frac{(-1)^n}{n!}\left(\frac{1}{\epsilon}+\psi(n+1)\right)+O(\epsilon), \tag{9.40}$$

for $n = 0, 1, 2, \ldots$, provides the next result.

Theorem 9.4.3. *The integrals $C_{3,k}$ are given by*

$$C_{3,k} = \frac{2}{3}\frac{1}{k!}\sum_{n=0}^{\infty}\frac{1}{(n!)^2}\frac{\Gamma\left(n+\frac{k+1}{2}\right)^4}{\Gamma(2n+k+1)}\left(\psi(n+1) - 2\psi\left(n+\tfrac{k+1}{2}\right) + \psi(2n+k+1)\right).$$

In particular, for $k = 1$

$$C_3 = \frac{2}{3}\sum_{n=0}^{\infty}\frac{(n!)^2}{(2n+1)!}\left(\psi(2n+2) - \psi(n+1)\right). \tag{9.41}$$

The evaluation of this sum using `Mathematica 7` yields a large collection of special values of (poly-)logarithms. After simplifications, it yields $C_3 = L_{-3}(2)$ as in (9.17).

Remark 9.4.4. An extension of Theorem 9.4.3 is presented next:

$$C_{3,k}(\alpha,\beta,\gamma) = \int_0^\infty\int_0^\infty\int_0^\infty \frac{x^{\alpha-1}y^{\beta-1}z^{\gamma-1}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{(x+1/x+y+1/y+z+1/z)^{k+1}}, \tag{9.42}$$

for $\gamma = 0$, is given by

$$\frac{1}{k!}\sum_{n=0}^{\infty}\frac{1}{(n!)^2}\frac{\Gamma\left(n+\frac{k+1\pm\alpha\pm\beta}{2}\right)}{\Gamma(2n+k+1)}\left(\psi(n+1) - \frac{1}{2}\psi\left(n+\tfrac{k+1\pm\alpha\pm\beta}{2}\right) + \psi(2n+k+1)\right)$$

where the notation $\Gamma(n+\frac{k+1\pm\alpha\pm\beta}{2}) = \Gamma(n+\frac{k+1+\alpha+\beta}{2})\Gamma(n+\frac{k+1+\alpha-\beta}{2})\cdots$ as well as $\psi(n+\frac{k+1\pm\alpha\pm\beta}{2}) = \psi(n+\frac{k+1+\alpha+\beta}{2}) + \psi(n+\frac{k+1+\alpha-\beta}{2}) + \cdots$ is employed. Similar expressions can be given for other integral values of γ. In the case where γ is not integral, $C_{3,k}(\alpha,\beta,\gamma)$ can be written as a sum of two ${}_3F_2$'s with Γ factors. The symmetry of $C_{3,k}(\alpha,\beta,\gamma)$ in α,β,γ, shows that this can be done if at least one of these arguments is nonintegral.

9.4.3 Evaluation of C_4

The last example discussed here is

$$C_4 = \frac{1}{6}\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty \frac{\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}w}{xyzw\,(x+1/x+y+1/y+z+1/z+w+1/w)^2}.$$

To minimize the number of sums and to maximize the number of brackets this is rewritten as

$$\frac{1}{6}\int_0^\infty\int_0^\infty\int_0^\infty\int_0^\infty \frac{x^{1+\epsilon}y^{1+\epsilon}z^{1+\epsilon}w^{1+\epsilon}\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{d}w}{[Axyzw(x+y)+zw(x+y)+xyzw(z+w)+xy(z+w)]^2}$$

with the intent of letting $\epsilon \to 0$ and $A \to 1$. As in the case of $C_{3,k}$, the *regulator* parameter ϵ is introduced to cure the divergence of the resulting expressions. Similarly, the parameter A is employed to divide the resulting sums into convergence groups according to the heuristic Rule 9.2.5. The denominator expands as

$$\sum_{\{n\}}\phi_{\{n\}}\; A^{n_1}x^{n_1+n_3+n_4}y^{n_1+n_3+n_4}z^{n_1+n_2+n_3}w^{n_1+n_2+n_3} \\ \times (x+y)^{n_1+n_2}(z+w)^{n_3+n_4}\,\langle 2+n_1+n_2+n_3+n_4\rangle\,.$$

As before,

$$(x+y)^{n_1+n_2} = \sum_{n_5,n_6}\phi_{n_5,n_6}\; x^{n_5}y^{n_6}\frac{\langle -n_1-n_2+n_5+n_6\rangle}{\Gamma(-n_1-n_2)}$$

and

$$(z+w)^{n_3+n_4} = \sum_{n_7,n_8}\phi_{n_7,n_8}\; z^{n_7}w^{n_8}\frac{\langle -n_3-n_4+n_7+n_8\rangle}{\Gamma(-n_3-n_4)}.$$

These expansions of the integrand yield the bracket series

$$\begin{aligned} \frac{1}{6} \sum_{\{n\}} \phi_{\{n\}} \, A^{n_1} \, \langle 2 + n_1 + n_2 + n_3 + n_4 \rangle \\ \times \; \frac{\langle -n_1 - n_2 + n_5 + n_6 \rangle}{\Gamma(-n_1 - n_2)} \frac{\langle -n_3 - n_4 + n_7 + n_8 \rangle}{\Gamma(-n_3 - n_4)} \\ \times \; \langle 2 + \epsilon + n_1 + n_3 + n_4 + n_5 \rangle \, \langle 2 + \epsilon + n_1 + n_3 + n_4 + n_6 \rangle \\ \times \; \langle 2 + \epsilon + n_1 + n_2 + n_3 + n_7 \rangle \, \langle 2 + \epsilon + n_1 + n_2 + n_3 + n_8 \rangle \, . \end{aligned} \tag{9.43}$$

The evaluation of this bracket series by Rules 9.2.4 and 9.2.5 yields hypergeometric series with arguments A (n_1, n_2, n_5, or n_6 chosen as the free index) and $1/A$ (n_3, n_4, n_7, or n_8 chosen as the free index). Either combination produces an expression for the integral C_4. Taking those with argument A (the indices n_5 and n_6 yield the same series; however, it is only taken into account once) gives

$$\begin{aligned} \frac{1}{12} A^{-\epsilon} \Gamma^2(\epsilon) \Gamma^2(1-\epsilon) \Bigg(\frac{A^{\epsilon}}{1+2\epsilon} {}_2F_1 \left(\left. \begin{matrix} \frac{1}{2} + \epsilon, 1 \\ \frac{3}{2} + \epsilon \end{matrix} \right| A \right) \\ + \frac{A^{-\epsilon}}{1-2\epsilon} {}_2F_1 \left(\left. \begin{matrix} \frac{1}{2} - \epsilon, 1 \\ \frac{3}{2} - \epsilon \end{matrix} \right| A \right) - 2 {}_2F_1 \left(\left. \begin{matrix} \frac{1}{2}, 1 \\ \frac{3}{2} \end{matrix} \right| A \right) \Bigg). \end{aligned} \tag{9.44}$$

As $\epsilon \to 0$, the limiting value is

$$\begin{aligned} \frac{1}{24} \ln^2 A \, \ln \left(\frac{1+\sqrt{A}}{1-\sqrt{A}} \right) + \frac{1}{3\sqrt{A}} \left[\mathrm{Li}_3(\sqrt{A}) - \mathrm{Li}_3(-\sqrt{A}) \right] \\ - \frac{\ln A}{6\sqrt{A}} \left[\mathrm{Li}_2(\sqrt{A}) - \mathrm{Li}_2(-\sqrt{A}) \right] . \end{aligned} \tag{9.45}$$

Finally, the value of C_4 is obtained by taking $A \to 1$:

$$C_4 = \frac{1}{3} \left[\mathrm{Li}_3(1) - \mathrm{Li}_3(-1) \right] = \frac{7}{12} \zeta(3). \tag{9.46}$$

This agrees with (9.17).

9.5 Analytic continuation of hypergeometric functions

The hypergeometric function ${}_pF_q$, defined by the series

$$ {}_pF_q(x) = {}_pF_q\left(\begin{matrix} a_1, \ldots, a_p \\ b_1, \ldots, b_q \end{matrix} \middle| x \right) = \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_p)_n}{(b_1)_n \cdots (b_q)_n} \frac{x^n}{n!}, \tag{9.47} $$

converges for all $x \in \mathbb{C}$ if $p < q+1$ and for $|x| < 1$ if $p = q+1$. In the remaining case, $p > q+1$, the series diverges for $x \neq 0$. The analytic continuation of the series ${}_{q+1}F_q$ has been recently considered in [Sko04a, Sko04b]. In this section a brackets representation of the hypergeometric series is obtained and then employed to produce its analytic extension.

Theorem 9.5.1. *The bracket representation of the hypergeometric function is given by*

$$ {}_pF_q(x) = \sum_{\substack{n \\ t_1,\ldots,t_p \\ s_1,\ldots,s_q}} \phi_{n,\{t\},\{s\}} \ \left[(-1)^{q-1}x\right]^n \prod_{j=1}^{p} \frac{\langle a_j + n + t_j \rangle}{\Gamma(a_j)} \prod_{k=1}^{q} \frac{\langle 1 - b_k - n + s_k \rangle}{\Gamma(1-b_k)}. $$

Proof. This follows from (9.47) and the representations

$$ (a_j)_n = \frac{\Gamma(a_j + n)}{\Gamma(a_j)} = \frac{1}{\Gamma(a_j)} \int_0^\infty \tau^{a_j+n-1} e^{-\tau} \, d\tau = \sum_{t_j} \phi_{t_j} \frac{\langle a_j + n + t_j \rangle}{\Gamma(a_j)} \tag{9.48} $$

as well as

$$ \frac{1}{(b_k)_n} = (-1)^n \frac{\Gamma(1 - b_k - n)}{\Gamma(1-b_k)} = (-1)^n \sum_{s_k} \phi_{s_k} \frac{\langle 1 - b_k - n + s_k \rangle}{\Gamma(1-b_k)} \tag{9.49} $$

for the Pochhammer symbol. □

The bracket expression for the hypergeometric function given in Theorem 9.5.1

contains $p+q$ brackets and $p+q+1$ indices (n, t_j and s_k). This leads to a full rank system

$$\begin{aligned} a_j + n + t_j &= 0 \qquad \text{for } 1 \leq j \leq p \\ 1 - b_k - n + s_k &= 0 \qquad \text{for } 1 \leq k \leq q. \end{aligned} \tag{9.50}$$

of linear equations of size $(p+q+1) \times (p+q)$ and determinant 1. For each choice of an index as a free variable the method of brackets yields a one-dimensional series for the integral.

Series with n as a free variable

Solving (9.50) yields $t_j^* = -a_j - n$ and $s_k^* = -(1-b_k) + n$ with $1 \leq j \leq p$ and $1 \leq k \leq q$. Rule 9.2.4 yields

$$\sum_{n=0}^{\infty} \frac{[(-1)^q x]^n}{n!} \prod_{j=1}^{p} \frac{\Gamma(n+a_j)}{\Gamma(a_j)} \prod_{k=1}^{q} \frac{\Gamma(-n+1-b_k)}{\Gamma(1-b_k)} = \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_p)_n}{(b_1)_n \cdots (b_q)_n} \frac{x^n}{n!}.$$

This is the original series representation (9.47) of the hypergeometric function. In particular, in the case $q = p-1$, this series converges for $|x| < 1$.

Series with t_i as a free variable

Fix an index i in the range $1 \leq i \leq p$ and solve (9.50) to get $n^* = -a_i - t_i$, as well as $t_j^* = t_i - a_j + a_i$ for $1 \leq j \leq p$, $j \neq i$, and $s_k^* = -(1-b_k) - a_i - t_i$ for $1 \leq k \leq q$. The method of brackets then produces the series

$$\sum_{t_i} \phi_{t_i} \left[(-1)^{q-1} x\right]^{-t_i - a_i} \frac{\Gamma(t_i + a_i)}{\Gamma(a_i)} \prod_{j \neq i} \frac{\Gamma(a_j - a_i - t_i)}{\Gamma(a_j)} \prod_{k} \frac{\Gamma(1 - b_k + a_i + t_i)}{\Gamma(1-b_k)}$$

which may be rewritten as

$$(-x)^{-a_i} \prod_{j \neq i} \frac{\Gamma(a_j - a_i)}{\Gamma(a_j)} \prod_{k} \frac{\Gamma(b_k)}{\Gamma(b_k - a_i)} \times {}_{q+1}F_{p-1}\left(\left. \begin{matrix} a_i, \{1 - b_k + a_i\}_{1 \leqslant k \leqslant q} \\ \{1 - a_j + a_i\}_{1 \leqslant j \leqslant p, j \neq i} \end{matrix} \right| \frac{(-1)^{p+q-1}}{x} \right). \tag{9.51}$$

Recall that the initial hypergeometric series ${}_pF_q(x)$ converges for some $x \neq 0$ if and only if $p \leqslant q+1$. Hence, assuming that $p \leqslant q+1$, observe that the hypergeometric series (9.51) converges for some x if and only if $p = q+1$.

Series with s_i as a free variable

Proceeding as in the previous case and choosing i in the range $1 \leq i \leq q$ and then s_i as the free index, gives

$$\left[(-1)^{p+q-1}x\right]^{1-b_i} \frac{\Gamma(b_i - 1)}{\Gamma(1 - b_i)} \prod_{j} \frac{\Gamma(1 - a_j)}{\Gamma(b_i - a_j)} \prod_{k \neq i} \frac{\Gamma(b_i - b_k)}{\Gamma(1 - b_k)} \times {}_pF_q\left(\left. \begin{matrix} \{a_j + 1 - b_i\}_{1 \leqslant j \leqslant p} \\ 2 - b_i, \{1 - b_k + b_i\}_{1 \leqslant k \leqslant q, k \neq i} \end{matrix} \right| x \right). \tag{9.52}$$

Summary

Assume $p = q+1$ and sum up the series coming from the method of brackets converging in the common region $|x| > 1$. Rule 9.2.5 gives the analytic continuation

$${}_{q+1}F_q(x) = \sum_{i=1}^{q+1} (-x)^{-a_i} \prod_{j \neq i} \frac{\Gamma(a_j - a_i)}{\Gamma(a_j)} \prod_{k} \frac{\Gamma(b_k)}{\Gamma(b_k - a_i)} \times {}_{q+1}F_q\left(\left. \begin{matrix} a_i, \{1 - b_k + a_i\}_{1 \leqslant k \leqslant q} \\ \{1 - a_j + a_i\}_{1 \leqslant j \leqslant q+1, j \neq i} \end{matrix} \right| \frac{1}{x} \right) \tag{9.53}$$

for the series (9.47).

On the other hand, the $q+1$ functions coming from choosing n or s_i, $1 \leqslant i \leqslant q$, as the free variables form linearly independent solutions to the hypergeometric differential equation

$$\prod_{j=1}^{q+1} \left(x \frac{\mathrm{d}}{\mathrm{d}x} + a_j \right) y = \prod_{k=1}^{q} \left(x \frac{\mathrm{d}}{\mathrm{d}x} + b_k \right) y \tag{9.54}$$

in a neighborhood of $x = 0$. Likewise, the $q+1$ functions (9.51) coming from choosing t_i, $1 \leqslant i \leqslant q+1$, as the free variables form linearly independent solutions to (9.54) in a neighborhood of $x = \infty$.

Example 9.5.2. For instance, if $p = 2$ and $q = 1$ then

$$\begin{aligned} {}_2F_1 \left(\left. \begin{matrix} a, b \\ c \end{matrix} \right| x \right) = (-x)^{-a} \frac{\Gamma(b-a)\Gamma(c)}{\Gamma(b)\Gamma(c-a)} {}_2F_1 \left(\left. \begin{matrix} a, 1-c+a \\ 1-b+a \end{matrix} \right| \frac{1}{x} \right) \\ + (-x)^{-b} \frac{\Gamma(a-b)\Gamma(c)}{\Gamma(a)\Gamma(c-b)} {}_2F_1 \left(\left. \begin{matrix} b, 1-c+b \\ 1-a+b \end{matrix} \right| \frac{1}{x} \right). \end{aligned} \tag{9.55}$$

This is entry 9.132.1 of [GR80]. On the other hand, the two functions

$${}_2F_1 \left(\left. \begin{matrix} a, b \\ c \end{matrix} \right| x \right), \qquad x^{1-c} {}_2F_1 \left(\left. \begin{matrix} a+1-c, b+1-c \\ 2-c \end{matrix} \right| x \right) \tag{9.56}$$

form a basis of the solutions to the second-order hypergeometric differential equation

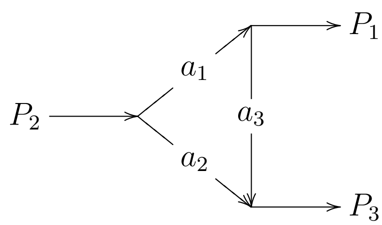
$$\left(x \frac{\mathrm{d}}{\mathrm{d}x} + a \right) \left(x \frac{\mathrm{d}}{\mathrm{d}x} + b \right) y = \left(x \frac{\mathrm{d}}{\mathrm{d}x} + c \right) y \tag{9.57}$$

in a neighborhood of $x = 0$.

9.6 Feynman diagram application

In Quantum Field Theory the permanent contrast between experimental measurements and theoretical models has been possible due to the development of novel and powerful analytical and numerical techniques in perturbative calculations. The fundamental problem that arises in perturbation theory is the actual calculation of the loop integrals associated to the Feynman diagrams, whose solution is specially difficult since these integrals contain in general both ultraviolet (UV) and infrared (IR) divergences. Using the dimensional regularization scheme, which extends the dimensionality of space-time by adding a fractional piece ($D = 4 - 2\epsilon$), it is possible to know the behavior of such divergences in terms of Laurent expansions with respect to the dimensional regulator ϵ when it tends to zero

As an illustration of the use of method of brackets, the Feynman diagram



(9.58)

considered in [BD91] is resolved. In this diagram the propagator (or internal line) associated to the index a_1 has mass m and the other parameters are $P_1^2 = P_3^2 = 0$ and $P_2^2 = (P_1 + P_3)^2 = s$. The D-dimensional representation in Minkowski space is given by

$$G = \int \frac{d^D q}{i\pi^{D/2}} \frac{1}{\left[(P_1+q)^2 - m^2\right]^{a_1} \left[(P_3-q)^2\right]^{a_2} \left[q^2\right]^{a_3}}. \tag{9.59}$$

In order to evaluate this integral, the Schwinger parametrization of (9.59) is considered (see [IZ93] for details). This is given by

$$G = \frac{(-1)^{-D/2}}{\prod_{j=1}^{3} \Gamma(a_j)} H \tag{9.60}$$

with H defined by

$$H = \int_0^\infty \int_0^\infty \int_0^\infty x_1^{a_1-1} x_2^{a_2-1} x_3^{a_3-1} \frac{\exp\left(x_1 m^2\right) \exp\left(-\frac{x_1 x_2}{x_1+x_2+x_3} s\right)}{\left(x_1+x_2+x_3\right)^{D/2}} \, dx_1 dx_2 dx_3. \tag{9.61}$$

To apply the method of brackets the exponential terms are expanded as

$$\exp\left(x_1 m^2\right)\exp\left(-\frac{x_1 x_2}{x_1+x_2+x_3}s\right) = \sum_{n_1,n_2} \phi_{n_1,n_2}\,(-1)^{n_1} m^{2n_1} s^{n_2} \frac{x_1^{n_1+n_2} x_2^{n_2}}{(x_1+x_2+x_3)^{n_2}},$$

and then (9.61) is transformed into

$$\sum_{n_1,n_2} \phi_{n_1,n_2}(-m^2)^{n_1} s^{n_2} \int_0^\infty\int_0^\infty\int_0^\infty \frac{x_1^{a_1+n_1+n_2-1} x_2^{a_2+n_2-1} x_3^{a_3-1}}{(x_1+x_2+x_3)^{D/2+n_2}}\, dx_1 dx_2 dx_3. \tag{9.62}$$

Further expanding

$$\frac{1}{(x_1+x_2+x_3)^{D/2+n_2}} = \sum_{n_3,n_4,n_5} \phi_{n_3,n_4,n_5}\, x_1^{n_3} x_2^{n_4} x_3^{n_5} \frac{\left\langle \frac{D}{2}+n_2+n_3+n_4+n_5 \right\rangle}{\Gamma(\frac{D}{2}+n_2)},$$

and replacing into (9.62) and substituting the resulting integrals by the corresponding brackets yields

$$\begin{aligned} H = &\sum_{\{n\}} \phi_{\{n\}}(-1)^{n_1} m^{2n_1} s^{n_2} \frac{\left\langle \frac{D}{2}+n_2+n_3+n_4+n_5 \right\rangle}{\Gamma(\frac{D}{2}+n_2)} \\ &\times\ \langle a_1+n_1+n_2+n_3\rangle \langle a_2+n_2+n_4\rangle \langle a_3+n_5\rangle . \end{aligned} \tag{9.63}$$

This bracket series is now evaluated employing Rules 9.2.4 and 9.2.5. Possible choices for free variables are n_1, n_2, and n_4. The series associated to n_2 converges for $|\frac{s}{m^2}| < 1$, whereas the series associated to n_1, n_4 converge for $|\frac{m^2}{s}| < 1$. The following two representations for G follow from here.

Theorem 9.6.1. *In the region* $|\frac{s}{m^2}| < 1$,

$$H = \eta_2 \cdot {}_2F_1\left(\left. \begin{matrix} a_1+a_2+a_3-\frac{D}{2}, a_2 \\ \frac{D}{2} \end{matrix} \right| \frac{s}{m^2} \right) \tag{9.64}$$

with η_2 defined by

$$\eta_2 = \left(-m^2\right)^{\frac{D}{2}-a_1-a_2-a_3} \frac{\Gamma(a_2)\Gamma(a_3)\Gamma\left(a_1+a_2+a_3-\frac{D}{2}\right)\Gamma\left(\frac{D}{2}-a_2-a_3\right)}{\Gamma\left(\frac{D}{2}\right)}.$$

Theorem 9.6.2. *In the region $|\frac{m^2}{s}| < 1$,*

$$H = \eta_1 \cdot {}_2F_1\left(\left.\begin{matrix} a_1+a_2+a_3-\frac{D}{2}, 1+a_1+a_2+a_3-D \\ 1+a_1+a_3-\frac{D}{2} \end{matrix}\right| \frac{m^2}{s}\right) \tag{9.65}$$
$$+ \eta_4 \cdot {}_2F_1\left(\left.\begin{matrix} 1+a_2-\frac{D}{2}, a_2 \\ 1-a_1-a_3+\frac{D}{2} \end{matrix}\right| \frac{m^2}{s}\right)$$

with η_1, η_4 defined by

$$\eta_1 = s^{\frac{D}{2}-a_1-a_2-a_3} \frac{\Gamma(a_3)\Gamma\left(a_1+a_2+a_3-\frac{D}{2}\right)\Gamma\left(\frac{D}{2}-a_1-a_3\right)\Gamma\left(\frac{D}{2}-a_2-a_3\right)}{\Gamma\left(D-a_1-a_2-a_3\right)},$$
$$\eta_4 = s^{-a_2}\left(-m^2\right)^{\frac{D}{2}-a_1-a_3} \frac{\Gamma(a_2)\Gamma(a_3)\Gamma\left(a_1+a_3-\frac{D}{2}\right)\Gamma\left(\frac{D}{2}-a_2-a_3\right)}{\Gamma\left(\frac{D}{2}-a_2\right)}.$$

These two solutions are now specialized to $a_1 = a_2 = a_3 = 1$. This situation is specially relevant, since when an arbitrary Feynman diagram is computed, the indices associated to the propagators are normally 1. Then, with $D = 4 - 2\epsilon$, the equations (9.64) and (9.65) take the form

$$H = (-m^2)^{-1-\epsilon}\Gamma(\epsilon-1){}_2F_1\left(\left.\begin{matrix} 1+\epsilon, 1 \\ 2-\epsilon \end{matrix}\right| \frac{s}{m^2}\right) \tag{9.66}$$

for $|\frac{s}{m^2}| < 1$, as well as

$$H = s^{-1-\epsilon}\frac{\Gamma(-\epsilon)^2\Gamma(1+\epsilon)}{\Gamma(1-2\epsilon)}\left(1-\frac{m^2}{s}\right)^{-2\epsilon} - m^{-2\epsilon}\frac{\Gamma(\epsilon)}{\epsilon s}{}_2F_1\left(\left.\begin{matrix} \epsilon, 1 \\ 1-\epsilon \end{matrix}\right| \frac{m^2}{s}\right) \tag{9.67}$$

for $|\frac{m^2}{s}| < 1$. Observe that these representations both have a pole at $\epsilon = 0$ of first order (for the second representation, each of the summands has a pole of second order which cancel each other).

9.7 Conclusions and future work

The method of brackets provides a very effective procedure to evaluate definite integrals over the interval $[0, \infty)$. The method is based on a heuristic list of rules on the bracket series associated to such integrals. In particular, a variety of examples that illustrate the power of this method has been provided. A rigorous validation of these rules as well as a systematic study of integrals from Feynman diagrams is in progress.

Chapter 10

A fast numerical algorithm for the integration of rational functions

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[MMMS10] *A fast numerical algorithm for the integration of rational functions*
(with Dante Manna, Luis Medina, Victor H. Moll)
published in Numerische Mathematik, Vol. 115, Nr. 2, Apr 2010, p. 289-307

Abstract A new iterative method for high-precision numerical integration of rational functions on the real line is presented. The algorithm transforms the rational integrand into a new rational function preserving the integral on the line. The coefficients of the new function are explicit polynomials in the original ones. These transformations depend on the degree of the input and the desired order of the method. Both parameters are arbitrary. The formulas can be precomputed. Iteration yields an approximation of the desired integral with m-th order convergence. Examples illustrating the automatic generation of these formulas and the numerical behaviour of this method are given.

10.1 Introduction

The numerical integration of the elliptic integral

$$G(a,b) = \int_0^{\pi/2} \frac{d\theta}{\sqrt{a^2\cos^2\theta + b^2\sin^2\theta}} \tag{10.1}$$

can be accomplished by iterating the transformation

$$\mathcal{L}_e : \mathbb{R}^2 \to \mathbb{R}^2, \quad (a,b) \mapsto \left(\frac{a+b}{2}, \sqrt{ab}\right). \tag{10.2}$$

Gauss [Gau99] established that $G(a,b)$ is invariant under the transformation $\mathcal{L}_e$, i.e.,

$$G(\mathcal{L}_e(a,b)) = G(a,b). \tag{10.3}$$

Moreover, the iterates (a_n, b_n) defined recursively by $(a_0, b_0) = (a, b)$ and $(a_n, b_n) = \mathcal{L}_e(a_{n-1}, b_{n-1})$ for $n \geq 1$, satisfy

$$|a_{n+1} - b_{n+1}| \leq \frac{1}{2}|a_n - b_n|^2, \tag{10.4}$$

illustrating the quadratic convergence of a_n and b_n to a common limit $\mathrm{AGM}(a,b)$. This is the *arithmetic-geometric* mean of a and b. $\mathcal{L}_e$ is known as the *elliptic Landen transformation*. The reader will find in [MM08a] a survey of the diverse aspects of this transformation and its generalizations.

The invariance of the integral $G(a,b)$ under $\mathcal{L}_e$ yields

$$G(a,b) = \frac{\pi}{2}\mathrm{AGM}^{-1}(a,b). \tag{10.5}$$

In particular, the value of the elliptic integral $G(a,b)$ can be approximated using the iterates a_n (or b_n). The functions $G(a,b)$ and $\mathrm{AGM}(a,b)$ along with the formula

(10.5), are at the center of highly effective computation of the basic constants of Analysis [BB98].

A scheme for the computation of the rational integral

$$F(a,b) = \int_{-\infty}^{\infty} \frac{b_0 x^{p-2} + \ldots + b_{p-3}x + b_{p-2}}{a_0 x^p + \ldots + a_{p-1}x + a_p}\, dx, \tag{10.6}$$

with $a = (a_0, a_1, \ldots, a_p)$, $b = (b_0, b_1, \ldots, b_{p-2})$, is presented here. *Rational Landen transformations*

$$\mathcal{L}_{m,p} : \mathbb{C}^{2p} \to \mathbb{C}^{2p}, \quad (a,b) \mapsto \mathcal{L}_{m,p}(a,b) \tag{10.7}$$

which preserve the integral $F(a,b)$ are constructed. Iteration of $\mathcal{L}_{m,p}$ yields a sequence of coefficients $(a_{n,0}, a_{n,1}, \cdots, a_{n,p})$ and $(b_{n,0}, b_{n,1}, \cdots, b_{n,p-2})$ for a sequence of rational functions which are shown to converge to a constant multiple of $1/(x^2+1)$. The invariance of the integral $F(a,b)$ under $\mathcal{L}_{m,p}$ yields

$$F(a,b) = c\int_{-\infty}^{\infty} \frac{dx}{x^2+1} = \pi c = \pi \lim_{n\to\infty} \frac{b_{n,0}}{a_{n,0}}, \tag{10.8}$$

that determines the constant c. The sequence $\{\pi b_{n,0}/a_{n,0} : \, n = 1, 2, 3 \ldots\}$ of approximations to the integral $F(a,b)$ converges with order m; that is, the error $e_n := |\pi b_{n,0}/a_{n,0} - F(a,b)|$ satisfies

$$|e_{n+1} - e_n| \leq C|e_n - e_{n-1}|^m \tag{10.9}$$

with an absolute constant C.

The outlined algorithm for computing rational integrals over the real line, presented in more detail in Section 10.6, consists of the two parts:

- **Creation** of the rational Landen transformation $\mathcal{L}_{m,p}$ where m is the desired order of convergence and p is the degree of the denominator of the rational function to be integrated. This is discussed in Section 10.2.

- **Iteration** of the Landen transformation, which is analyzed in Sections 10.3 and 10.6 with the view towards complexity and implementation, respectively.

Numerical examples of this method are discussed in Section 10.4.

Remark 10.1.1. Given m and p, the map $\mathcal{L}_{m,p}$ can be *precomputed* and the result can be stored for use in the second part of the algorithm. Therefore, the first part of the algorithm carries a *one-time cost* and is not figured into the complexity of the method which is discussed in Section 10.3.

Remark 10.1.2. The numerical method for the integration of rational functions presented here is different in spirit than the standard ones: the approximation to the integral is obtained from a *recurrence* acting on the coefficients of the integrand. In particular, the domain of integration is not discretized and the integrand is never evaluated. Examples that illustrate the method and a study of the cost involved are presented.

Future work. The algorithm presented here is restricted to integrals on the whole line. The extension to a finite interval requires the development of Landen transformations on the half line. This question is open, even for the simplest case of

$$I_2(a,b,c) := \int_0^\infty \frac{dx}{ax^2+bx+c}. \tag{10.10}$$

The method has been coupled with Pade approximations [BCGK+10] to produce a fast, robust integration algorithm for some non-rational integrands; namely, those of the form $R(\mu(x))\mu'(x)$ for a rational function R and an increasing change of scale μ. Extensions to all smooth integrands remain to be completed.

10.2 The Landen transformation

In this section we present simple examples, and then describe the algorithm in detail. The first two examples show the transformations $\mathcal{L}_{2,2}$ and $\mathcal{L}_{3,4}$. Both maps are given by polynomial functions.

Example 10.2.1. The rational Landen transformation $\mathcal{L}_{2,2}$ is given by

$$\mathcal{L}_{2,2}(b_0, a_0, a_1, a_2) = (b_0', a_0', a_1', a_2'),$$

with

$$\begin{aligned} b_0' &= 2a_0b_0 + 2a_2b_0, \\ a_0' &= 4a_0a_2, \\ a_1' &= -2a_0a_1 + 2a_1a_2, \\ a_2' &= a_0^2 - a_1^2 + 2a_0a_2 + a_2^2. \end{aligned}$$

Example 10.2.2. The rational Landen transformation $\mathcal{L}_{3,4}$ is computed as

$$\mathcal{L}_{3,4}(b_0, b_1, b_2, a_0, a_1, a_2, a_3, a_4) = (b_0', b_1', b_2', a_0', a_1', a_2', a_3', a_4')$$

with

$$\begin{aligned} b_0' &= 3a_0^2b_0 - a_1^2b_0 + 10a_0a_2b_0 + 3a_2^2b_0 - 6a_1a_3b_0 - 9a_3^2b_0 + \ldots \\ a_0' &= a_0^3 - 3a_0a_1^2 + 6a_0^2a_2 + 9a_0a_2^2 - 18a_0a_1a_3 - 27a_0a_3^3 + 18a_0^2a_4 + \ldots \end{aligned}$$

and so on. The point to be made here is that, while the formulas for the transformations $\mathcal{L}_{m,p}$ grow in size as m and p increase, these formulas only have to be computed once.

Remark 10.2.3. The rational Landen transformations $\mathcal{L}_{m,p}$ are given by polynomial equations which are homogeneous of degree m. Furthermore, the a_i' depend only on the a_i.

Remark 10.2.4. The invariance of $F(a,b)$ under $\mathcal{L}_{m,p}$ implies that the set

$$\mathcal{R} = \{(a,b) \in \mathbb{R}^{2p} : \quad F(a,b) \text{ is finite}\} \tag{10.1}$$

is preserved by $\mathcal{L}_{m,p}$. The action of $\mathcal{L}_{m,p}$ outside of $\mathcal{R}$ is difficult to analyze. The reader will find in [Mol02] some illustrations for $\mathcal{L}_{2,6}$.

Remark 10.2.5. The dynamical study of $\mathcal{L}_{2,6}$ appeared in [CM06]. An extension of this work to $\mathcal{L}_{3,6}$ and $\mathcal{L}_{4,6}$ will appear in [CEK$^+$10] and [GNO$^+$10], respectively.

Example 10.2.6. Iterating $\mathcal{L}_{2,2}$ with initial conditions $a_{0,i} = a_i$, $b_{0,i} = b_i$ yields a sequence $(b_{n,0}, a_{n,0}, a_{n,1}, a_{n,2})$, defined by

$$(b_{n+1,0}, a_{n+1,0}, a_{n+1,1}, a_{n+1,2}) := \mathcal{L}_{2,2}(b_{n,0}, a_{n,0}, a_{n,1}, a_{n,2}),$$

which satisfies

$$\int_{-\infty}^{\infty} \frac{b_{n,0}\, dx}{a_{n,0}x^2 + a_{n,1}x + a_{n,2}} = \int_{-\infty}^{\infty} \frac{b_0\, dx}{a_0x^2 + a_1x + a_2}.$$

The convergence result in Section 10.5 shows that

$$\frac{b_{n,0}}{a_{n,0}x^2 + a_{n,1}x + a_{n,2}} \sim \frac{b_{n,0}}{a_{n,0}} \frac{1}{x^2+1}$$

as $n \to \infty$. Furthermore the convergence is quadratic. Therefore,

$$\int_{-\infty}^{\infty} \frac{b_0\, dx}{a_0x^2 + a_1x + a_2} = \pi \lim_{n\to\infty} \frac{b_{n,0}}{a_{n,0}}.$$

For instance, starting with $1/(x^2+4x+15)$, the algorithm produces $\mathcal{L}_{2,2}(1,1,4,15) = (32, 60, 112, 240)$. Hence,

$$\int_{-\infty}^{\infty} \frac{dx}{x^2+4x+15} = \int_{-\infty}^{\infty} \frac{32\,dx}{60x^2+112x+240}.$$

The first two terms of the approximating sequence $I_n = \pi a_{n,0}/b_{n,0}$ are given by $I_0 = \pi$ and $I_1 = 32\pi/60$. These approximations converge to $\pi/\sqrt{11}$, the exact value of the integral. The error $e_n := |I_n - \pi/\sqrt{11}|$ and the relative approximate error $d_n := |(I_{n+1} - I_n)/I_{n+1}|$ are given in Table 10.1. Observe that 19 iterations provide about 100,000 correct digits. Furthermore, this precision can be reached by using just slightly more, say 5, than 100,000 digits of working precision.

n	1	2	3	4	5	10	20
e_n	0.73	0.10	0.034	0.00042	$1.2 \cdot 10^{-6}$	$7.8 \cdot 10^{-197}$	$7.0 \cdot 10^{-200,886}$
d_n	0.60	0.15	0.036	0.00044	$1.3 \cdot 10^{-6}$	$8.2 \cdot 10^{-197}$	$7.4 \cdot 10^{-200,886}$

Table 10.1: Absolute and relative approximate errors for a method of order 2.

The creation of the rational Landen transformation formulas depends on two polynomial sequences. Let $m \geq 2$ be an integer. Define the polynomials

$$\begin{aligned} P_m(x) &= \sum_{j=0}^{\lfloor m/2 \rfloor} (-1)^j \binom{m}{2j} x^{m-2j} \\ Q_m(x) &= \sum_{j=0}^{\lfloor (m-1)/2 \rfloor} (-1)^j \binom{m}{2j+1} x^{m-(2j+1)}, \end{aligned} \tag{10.2}$$

that come from the relation

$$\cot(m\theta) = R_m(\cot\theta) \tag{10.3}$$

satisfied by $R_m = P_m/Q_m$. Details about these polynomials can be found in [MM07].

Let A, B be polynomials. The change of variables $y = R_m(x)$ yields a new pair of polynomials A_1, B_1 such that

$$\int_{-\infty}^{\infty} \frac{B_1(x)}{A_1(x)} dx = \int_{-\infty}^{\infty} \frac{B(x)}{A(x)} dx. \tag{10.4}$$

The change of variables requires the domain to be splitted according to the branches of the inverse R_m^{-1}. These are specified by the intervals (q_{j-1}, q_j) where $q_0 = -\infty$, $q_j = \cot(\pi j/m)$ for $1 \leq j \leq m-1$, and $q_m = +\infty$. The function $y = R_m(x)$ is invertible on each of the subintervals (q_{j-1}, q_j), and the (local) inverse is denoted by $x = \omega_j(y)$. After substituting $y = R_m(x)$ in each interval, it follows that

$$\int_{-\infty}^{\infty} \frac{B(x)}{A(x)} dx = \sum_{j=1}^{m} \int_{q_{j-1}}^{q_j} \frac{B(x)}{A(x)} dx = \int_{-\infty}^{\infty} \sum_{j=1}^{m} \frac{B(\omega_j(y))}{A(\omega_j(y))} \omega_j'(y) dy. \tag{10.5}$$

The integrand on the right-hand side of (10.5) is indeed a rational function B_1/A_1; see [MM07]. The rational Landen transformation $\mathcal{L}_m : \mathbb{C}(x) \to \mathbb{C}(x)$ is defined by $B/A \mapsto B_1/A_1$. The full details are given below.

Step 1 The rational function $R_m = P_m/Q_m$ comes from (10.2). First construct the polynomial

$$A_1(x) := \operatorname{Res}\left(A, P_m - xQ_m\right)$$

where Res denotes the *resultant*. The degrees of the polynomials involved are $p := \deg A$ and $m = \deg(P_m - x\,Q_m)$, respectively. The degree of the denominator is preserved; that is, $\deg(A_1) = \deg(A)$. The coefficients of A_1 are polynomials in those of A.

Step 2 The polynomial $E_m(x) := [P_m(x)]^p \, A_1(R_m(x))$ is a multiple of A. Compute the quotient

$$C(x) := E(x)\frac{B(x)}{A(x)} = \sum_{k=0}^{s} c_k x^{s-k},$$

with $s := mp - 2$.

Step 3 Define the expressions

$$
\begin{aligned}
T_x(a,b) &:= \sum_{j=0}^{x} (-1)^{a-x+j} \binom{a}{x-j}\binom{b}{j}, \\
M_1(j,\alpha,\beta,\gamma) &:= (-1)^{j+\alpha-\beta} c_{2j} \frac{2^{2(\alpha-\beta)}\alpha}{2\alpha-\beta} \binom{2\alpha-\beta}{\beta}\binom{\nu-\alpha-1+\beta}{\gamma} \times \\
&\quad\ (T_{\lambda+\alpha m}(2j, s-2j) + T_{\lambda-\alpha m}(2j, s-2j)), \\
M_2(j,\alpha,\beta,\gamma) &:= (-1)^{j+\beta} c_{2j+1} 2^{2\beta+1} \binom{\alpha+\beta}{2\beta+1}\binom{\nu-2-\beta}{\gamma} \times \\
&\quad\ (T_{\lambda+\alpha m}(2j+1, s-2j-1) - T_{\lambda-\alpha m}(2j+1, s-2j-1)),
\end{aligned}
$$

where $\nu := p/2$ and $\lambda := (mp-2)/2$.

Step 4 Define

$$
\begin{aligned}
B_1(x) &:= \frac{1}{2^s} \sum_{\gamma=0}^{\nu-1} \left(\binom{\nu-1}{\gamma} \sum_{j=0}^{\lambda} (-1)^j c_{2j} T_\lambda(2j, s-2j) \right) x^{2\gamma} \\
&+ \frac{1}{2^s} \sum_{\gamma=0}^{\nu-2} \left(\sum_{j=0}^{\lambda} \sum_{\alpha=1}^{\nu-1-\gamma} \sum_{\beta=0}^{\alpha} M_1(j,\alpha,\beta,\gamma) \right) x^{2\gamma} \\
&+ \frac{1}{2^s} \sum_{\gamma=1}^{\nu-1} \left(\sum_{j=0}^{\lambda} \sum_{\alpha=\nu-\gamma}^{\nu-1} \sum_{\beta=\alpha-\nu+\gamma+1}^{\alpha} M_1(j,\alpha,\beta,\gamma) \right) x^{2\gamma} \\
&+ \frac{1}{2^s} \sum_{\gamma=0}^{\nu-2} \left(\sum_{j=0}^{\lambda-1} \sum_{\alpha=1}^{\nu-1-\gamma} \sum_{\beta=0}^{\alpha-1} M_2(j,\alpha,\beta,\gamma) \right) x^{2\gamma+1} \\
&+ \frac{1}{2^s} \sum_{\gamma=1}^{\nu-2} \left(\sum_{j=0}^{\lambda-1} \sum_{\alpha=\nu-\gamma}^{\nu-1} \sum_{\beta=0}^{\alpha-1} M_2(j,\alpha,\beta,\gamma) \right) x^{2\gamma+1}.
\end{aligned}
$$

The following theorem has been established in [MM07].

Theorem 10.2.7. *The rational function B_1/A_1 satisfies*

$$
\int_{-\infty}^{\infty} \frac{B_1(x)}{A_1(x)} dx = \int_{-\infty}^{\infty} \frac{B(x)}{A(x)} dx \tag{10.6}
$$

whenever one of the integrals is finite. Moreover $\deg A_1 = \deg A$.

Definition 10.2.8. The *rational Landen transformation* $\mathcal{L}_m : \mathbb{C}(x) \to \mathbb{C}(x)$ is defined by $\mathcal{L}_m(B/A) = B_1/A_1$. When $\mathcal{L}_m$ is acting on the coefficients of a rational function of degree p we write $\mathcal{L}_{m,p}(b_0, b_1, \ldots, b_{p-2}, a_0, a_1, \ldots, a_p)$ as in (10.7) and Example 10.2.6.

Precomputed formulas for the $\mathcal{L}_{m,p}$ as well as a program written in Mathematica that generates these formulas following the above algorithm and featuring the numerical integration of rational functions over the real line, as outlined in the introduction, are available for download from the authors. Some details of the implementation will be discussed in Section 10.6.

10.3 Complexity of the algorithm

This section discusses the complexity of computing definite integrals using Landen transformations. The analysis is restricted to the cost of one iteration. The actual generation of the Landen transformation is not considered since it is a one-time cost.

Examples 10.2.1 and 10.2.2 illustrate the fact that $\mathcal{L}_{m,p}$ is a mapping $\mathbb{C}^{2p} \to \mathbb{C}^{2p}$ defined by polynomial equations with integer coefficients. Assume that these polynomial equations appear in expanded form. The number of multiplications $c_{m,p}$ involved in computing $\mathcal{L}_{m,p}$ not including multiplications with constants is now counted. Additions and multiplying with constants have lower complexity than multiplication which is why they are not included in this count.

Example 10.3.1. Example 10.2.1 gives $\mathcal{L}_{2,2}(b_0, a_0, a_1, a_2) = (b_0', a_0', a_1', a_2')$ with

$$\begin{aligned} b_0' &= 2a_0b_0 + 2a_2b_0, \\ a_0' &= 4a_0a_2, \\ a_1' &= -2a_0a_1 + 2a_1a_2, \\ a_2' &= a_0^2 - a_1^2 + 2a_0a_2 + a_2^2. \end{aligned}$$

Hence $\mathcal{L}_{2,2}$ requires $c_{2,2} = 9$ multiplications. More values $c_{m,p}$ are given in Table 10.2.

$p\backslash m$	2	3	4	5
2	9	32	75	144
4	36	204	702	1896
6	94	756	3492	12040
8	195	2056	11895	49712
10	351	4600	31923	156512
12	574	9012	72858	409688

Table 10.2: Number of operations involved in $\mathcal{L}_{m,p}$.

The data above suggest that $c_{m,p} = O(p^{m+1})$. Moreover, for $m = 2$ and $m = 3$ the number of multiplications $c_{m,2p}$ seem to be *exactly*

$$c_{2,2p} = \frac{1}{2}(p+1)\left(2 + 3p + 4p^2\right), \tag{10.1}$$

$$c_{3,2p} = \frac{2}{3}p\left(15 + 13p + 12p^2 + 8p^3\right). \tag{10.2}$$

Remark 10.3.2. As noted in Remark 10.2.3, the Landen transformation $\mathcal{L}_{m,p}$ only involves monomials of degree m. Therefore, $c_{m,p}$ is the number of these monomials times $m-1$. Writing the polynomial expressions defining $\mathcal{L}_{m,p}$ in a different form, one may hope to decrease the cost of its computation. Experiments conducted in Mathematica show that writing these polynomials in multivariate Horner form decreases the order of growth to $O(p^m)$.

Remark 10.3.3. From a practical point of view, the Landen transformations of order 2 are generally preferable to higher order ones. This is because combining n Landen iterations $\mathcal{L}_{2,p}$ into one step gives a method of order 2^n (in fact, $\mathcal{L}_{2,p}^n = \mathcal{L}_{2^n,p}$) which requires $nc_{2,p}$ multiplications. Multiple experiments show that $nc_{2,p} \ll c_{2^n,p}$.

10.4 Some numerical examples

In this section two examples that illustrate the procedure described in this work are presented.

Example 10.4.1. This first example illustrates the behavior on highly oscillatory integrands which, as it turns out, is basically no different from the behaviour on more regular integrands. A Landen transformation of order 2 is applied to the rational function

$$f_k(x) = \frac{2^k P_k(x/2)}{\binom{k}{\lfloor k/2 \rfloor}(x^{2k}+1)}, \tag{10.1}$$

where P_k is the Legendre polynomial. The normalization factor is chosen so that $|f_k(0)| = 1$ for even k.

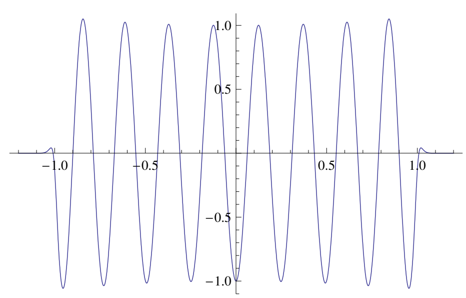


Figure 10.1: The oscillatory rational function $f_{50}(x)$

The number of steps $n_k(d)$ needed for the relative error to drop below 10^{-d} is tabulated in Table 10.3. These calculations only require a working precision of a few more, say 5, than d digits. Observe that, as expected, to obtain the 10 fold precision only about $\log(2,10) \approx 3.32$ additional iterations are necessary.

k	2	4	6	8	10	20	30	40	50
$n_k(20)$	6	7	8	8	9	10	10	11	11
$n_k(50)$	8	9	9	10	10	11	12	12	12
$n_k(100)$	9	10	10	11	11	12	13	13	13
$n_k(1000)$	12	13	14	14	14	15	16	16	17
$n_k(10000)$	15	16	17	17	18	19	19	20	20

Table 10.3: Number of steps $n_k(d)$ needed to get relative error less than 10^{-d}.

Example 10.4.2. The method proposed here is also applicable to problems that are nearly singular, that is, to rational functions with poles arbitrarily close to the real axis. For fixed $\epsilon > 0$, apply $\mathcal{L}_{2,2}$ to the rational function

$$f_\epsilon(x) = \frac{1}{(x-1)^2+\epsilon^2} = \frac{1}{x^2-2x+(1+\epsilon^2)} \tag{10.2}$$

which over the real line integrates to $1/\epsilon$. For decreasing values of $\epsilon = 10^{-k}$ the number of steps $n_k(d)$ needed so that the relative error is less than 10^{-d} can be found in Table 10.4. In this case, it is sufficient to use a working precision of $d + 2k$. The data in Table 10.4 suggest that the number of steps $n_k(d)$ grows linear in k and, as expected, logarithmic in d.

k	1	2	3	4	5	10	20	40
$n_k(20)$	9	13	16	19	23	39	72	139
$n_k(50)$	11	14	17	21	24	41	74	140
$n_k(100)$	12	15	18	22	25	42	75	141
$n_k(1000)$	15	18	22	25	28	45	78	145
$n_k(10000)$	18	22	25	28	32	48	81	148

Table 10.4: Number of steps $n_k(d)$ needed to get relative error less than 10^{-d} when integrating $f_{10^{-k}}$.

10.5 Convergence of Landen iterates

In this section the convergence of the iterates of the Landen transformation $\mathcal{L}_{m,p}$ starting at the rational function

$$f(x) = \frac{B(x)}{A(x)} = \frac{b_0 x^{p-2} + \ldots + b_{p-3}x + b_{p-2}}{a_0 x^p + \ldots + a_{p-1}x + a_p}$$

is considered. Denote by $f_n = B_n/A_n$ the Landen iterates $\mathcal{L}_{m,p}^n(f)$. Assuming that f has no poles on the real line, Theorem 10.5.7 shows that, as $n \to \infty$,

$$f_n \to \frac{c}{x^2+1}, \tag{10.1}$$

where c is determined by the integral of f (and vice versa). Moreover, convergence is of order m. This implies the convergence of the coefficients of $A_n = a_{n,0}x^p + a_{n,1}x^{p-1} + \ldots + a_{n,p}$ and $B_n = b_{n,0}x^{p-2} + b_{n,1}x^{p-3} + \ldots + b_{n,p-2}$ as described in the following proposition.

Proposition 10.5.1. *Let λ_+ be the number of roots of A with positive imaginary part and λ_- the number of roots with negative imaginary part (note that $\lambda_+ + \lambda_-$ is the degree of A). Then for the constant c defined in (10.1)*

$$\frac{B_n}{a_{n,0}} \to c(x-i)^{\lambda_+-1}(x+i)^{\lambda_--1}, \quad \frac{A_n}{a_{n,0}} \to (x-i)^{\lambda_+}(x+i)^{\lambda_-}.$$

Note that the constant c in (10.1) vanishes if either $\lambda_+ = 0$ or $\lambda_- = 0$.

Proof. The proof is given for $m = 2$, the general case can be established by similar methods. Recall that the denominator A_n only depends on A and it is transformed according to

$$A_{n+1}(x) = \mathrm{Res}_z(A_n(z), z^2 - 2xz - 1). \tag{10.2}$$

Hence, if $A_n/a_{n,0} = \prod_k (x - \lambda_{n,k})$ then

$$A_{n+1}/a_{n,0} = \prod_k \left(\lambda_{n,k}^2 - 2\lambda_{n,k}x - 1 \right).$$

Therefore the roots of $A_{n+1}(x)$ are $\lambda_{n+1,k} = \frac{\lambda_{n,k}^2 - 1}{2\lambda_{n,k}}$. Note that

$$\operatorname{Im}\left(\frac{\lambda^2 - 1}{2\lambda} \right) = \frac{1}{2}\left(1 + \frac{1}{|\lambda|^2} \right) \operatorname{Im}(\lambda),$$

which implies that the signs of the imaginary part of the roots of A are preserved by the Landen iterations. In particular, this shows that the integrablity of a rational function is preserved by $\mathcal{L}_{m,p}$.

The transformation $\lambda \mapsto \dfrac{\lambda^2 - 1}{2\lambda} = \lambda - \dfrac{\lambda^2 + 1}{2\lambda}$ is the Newton map of $\lambda^2 + 1$. Therefore, each root $\lambda_{n,k}$ converges to i or $-i$ depending on the sign of Im $\lambda_{1,k}$. Furthermore, the Newton map is known to exhibit quadratic convergence. This establishes the result about A_n. Theorem 10.5.7 shows that $B_n/A_n \to c/(x^2+1)$. This gives the corresponding result for B_n. □

Corollary 10.5.2. *If A has only real coefficients, then p is even and*

$$\frac{B_n}{a_{n,0}} \to c(x^2+1)^{p/2-1}, \quad \frac{A_n}{a_{n,0}} \to (x^2+1)^{p/2}.$$

Remark 10.5.3. An explicit and curious formula for the denominator A_1 of $\mathcal{L}_2(1/A)$ is described next. This is an expression independent of the roots of A. In the computation of $A_1(x) = \operatorname{Res}_z(A(z), z^2 - 2xz - 1)$, reduce $A(z)$ modulo $z^2 - 2xz - 1$ before computing the resultant. Proceeding in a recursive manner, write $z^n \equiv a_n(x) + b_n(x)z$. Then $z^2 \equiv 1 + 2xz$ leads to the recurrence

$$a_{n+1}(x) = b_n(x), \quad b_{n+1}(x) = a_n(x) + 2xb_n(x).$$

Therefore $z^n \equiv b_{n-1}(x) + b_n(x)z$ where $b_n(x)$ is defined by

$$b_{n+1}(x) = 2xb_n(x) + b_{n-1}(x), \quad b_0 = 0,\ b_1 = 1. \tag{10.3}$$

It follows that $z^n \equiv F_{n-1}(2x) + F_n(2x)z$ where $F_n(x)$ is the nth *Fibonacci polynomial*. These polynomials are defined recursively by $F_0(x) = 0$, $F_1(x) = 1$ and $F_{n+1}(x) = xF_n(x) + F_{n-1}(x)$ and they are explicitely given by

$$F_{n+1}(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n-k}{k} x^{n-2k}.$$

If $A(z) = \sum a_k z^k$ then $A(z) \equiv a(x) + b(x)z$ for $a(x) = \sum a_k F_{k-1}(2x)$ and $b(x) = \sum a_k F_k(2x)$. It follows that

$$\begin{aligned} A_1(x) &= a(x)^2 - b(x)^2 + 2a(x)b(x)x \\ &= a(x)(a(x) + 2xb(x)) - b(x)^2 \\ &= \left(\sum a_k F_{k-1}\right)\left(\sum a_k F_{k+1}\right) - \left(\sum a_k F_k\right)^2 \end{aligned}$$

where F_k is used to abbreviate $F_k(2x)$.

Remark 10.5.4. The proof of Proposition 10.5.1 contains explicitly the transformation of the denominator under the Landen transformation $\mathcal{L}_2$ in terms of its roots. In particular,

$$\mathcal{L}_2\left(\frac{1}{x-\lambda}\right) = \frac{-2\lambda}{-2\lambda x + \lambda^2 - 1} = \frac{1}{x - \frac{\lambda^2-1}{2\lambda}}.$$

For a rational function $f = B/A$, with no repeated poles off the real line and $\deg(B) \leq \deg(A) - 2$ (for integrability), consider the partial fraction decomposition $f = \sum_k b_k/(x - \lambda_k)$. Then, by linearity of $\mathcal{L}_2$,

$$\mathcal{L}_2(f) = \mathcal{L}_2\left(\sum_k \frac{b_k}{x-\lambda_k}\right) = \sum_k \frac{b_k}{x - \frac{\lambda_k^2-1}{2\lambda_k}}.$$

Assume that the poles of $\mathcal{L}_2^n(f)$ remain simple. Then

$$\mathcal{L}_2^n f \to \sum_k \frac{b_k}{x - \lambda_{\infty,k}}$$

where $\lambda_{\infty,k}$ is either i or $-i$ depending on the sign of Im λ_k. Thus, for some constants $c_\pm$,

$$\mathcal{L}_2^n f \to \frac{c_+}{x-i} + \frac{c_-}{x+i} = \frac{c}{x^2+1},$$

where the last equality follows from Theorem 10.2.7 and the fact that a Landen transformation preserves integrability.

The general proof requires some machinery from complex analysis. To this end, identify the integral of the rational function $f = B/A$ over the real line with the integral of the holomorphic 1-form $\phi = f(z)dz$ over the real projective line $\mathbb{R}P^1$; that is,

$$\int_{-\infty}^{\infty} f(x)dx = \int_{\mathbb{R}P^1} \phi,$$

where $\mathbb{R}P^1$ is the completed real axis sitting inside the Riemann sphere $\mathbb{C}P^1$. Recall that f being a rational function corresponds to a holomorphic function on $\mathbb{C}P^1$.

The next required concept is that of a *pull-back* of a holomorphic 1-form. After the definition, recall the change of variables formula that connects the integral of a 1-form to that of its pull-back. The reader will find all these concepts in [Sha94].

Definition 10.5.5. Let ϕ be a 1-form on a Riemann surface S, and $\pi : S \to T$ a holomorphic mapping between Riemann surfaces. The *pull-back* of ϕ induced by π is defined as

$$\pi_* \phi|_U = \sum_{i=1}^{k} \sigma_i^* \phi,$$

on all $U \subset T$ simply connected and containing no critical values of π. Here $\sigma_1, ..., \sigma_k : U \to S$ are the distinct sections of π.

It is an elementary consequence of this definition that for holomorphic mappings $\pi_1 : S_2 \mapsto S_3$ and $\pi_2 : S_1 \mapsto S_2$,

$$\pi_{1*}\pi_{2*}\phi = (\pi_1 \circ \pi_2)_*\phi$$

for any 1-form ϕ on S_1. The next lemma concerning holomorphic pull-backs and their path integrals is again an immediate consequence of the definition.

Lemma 10.5.6. *If $\pi : S \to T$ is a holomorphism of Riemann surfaces, and ϕ is a holomorphic 1-form on S, then $\pi_*\phi$ is a holomorphic 1-form on T. Furthermore, for any oriented rectifiable curve γ on T, the identity*

$$\int_\gamma \pi_*\phi = \int_{\pi^{-1}\gamma} \phi \tag{10.4}$$

holds.

Let $f = B/A$ be a rational function. The pull-back of the 1-form $\phi = f(z)dz$ on $\mathbb{C}P^1$ induced by $R_m : \mathbb{C}P^1 \to \mathbb{C}P^1$ is the 1-form

$$(R_m)_*\phi = \sum_{j=1}^{m} \frac{B(\omega_j(y))}{A(\omega_j(y))}\omega_j'(y)dy.$$

Note that the right-hand side of (10.5) is precisely the integral of $(R_m)_*\phi$ over the projective real line. In this case, Lemma 10.5.6 amounts to (10.5). The map $\mathcal{L}_m$ may therefore be identified with $(R_m)_*$. The following is a restatement of (10.1).

Theorem 10.5.7. *Let ϕ be a holomorphic 1-form in a neighborhood U of $\mathbb{R}P^1 \subset \mathbb{C}P^1$. Then*

$$\lim_{n\to\infty} (R_m)_*^n\phi = \frac{1}{\pi}\left(\int_{\mathbb{R}P^1} \phi\right)\frac{dz}{z^2+1}$$

where the convergence is of order m and uniform on compact subsets of U.

Remark 10.5.8. Let $f = B/A$ be a rational function such that its integral over the real line is finite. Then the 1-form $f(z)dz$ on $\mathbb{C}P^1$ is holomorphic on some open set $U \supset \mathbb{R}P^1$. In particular, for $\beta = \min\{|\operatorname{Im} x| : A(x) = 0\}$, and $N = \max\{|x| : A(x) = 0\}$, $f(z)dz$ is holomorphic on

$$V_\epsilon = \{x \in \mathbb{C}P^1 : |\operatorname{Im} x| < \beta - \epsilon\} \cup \{x \in \mathbb{C}P^1 : |x| > N + \epsilon\}$$

for all $\epsilon < \beta$.

A statement equivalent to Theorem 10.5.7 is proved now. This follows from conjugation by the map $M(z) = \frac{z+i}{z-i}$. Recall that $R_m = M^{-1} \circ f_m \circ M$, see for instance [MM07], where $f_m(z) = z^m$, so that $R_m^n = M^{-1} \circ f_m^n \circ M$ and therefore

$$\lim_{n\to\infty} (R_{m*})^n \phi = M_*^{-1} \lim_{n\to\infty} (f_{m*})^n \phi_1$$

where $\phi_1 = M_* \phi$. On the other hand, one verifies that

$$M_* \frac{dz}{z^2+1} = -\frac{dz}{2iz}.$$

Finally, observe that, by Lemma 10.5.6,

$$\int_{\mathbb{R}P^1} \phi = \int_{\mathbb{R}P^1} M_*^{-1} \phi_1 = -\int_{S^1} \phi_1$$

where S^1 denotes the path that rotates once around the unit circle in counterclockwise direction. Theorem 10.5.7 is therefore equivalent to the following statement.

Theorem 10.5.9. *Let ϕ be a holomorphic 1-form in a neighborhood U of S^1. Then*

$$\lim_{n\to\infty} (f_m)_*^n \phi = \frac{1}{2\pi i} \left(\int_{S^1} \phi \right) \frac{dz}{z}$$

where the convergence is of order m and uniform on compact subsets of U.

Proof. Using the local coordinate z, write $\phi = \phi(z)dz$ where $\phi(z)$ is analytic on an annulus $\frac{1}{R} < |z| < R$ for some $R > 1$. The function $\phi(z)$ admits a Laurent expansion

$$\phi(z) = \sum_{k=-\infty}^{\infty} a_k z^k$$

and the coefficients a_k satisfy

$$\|\phi\| := \sum_{k=-\infty}^{\infty} |a_k| R^{|k|} < \infty.$$

Since

$$a_{-1} = \frac{1}{2\pi i} \int_{S^1} \phi(z)dz$$

it is required to show that

$$\lim_{n\to\infty} (f_m)_*^n \phi = a_{-1} \frac{dz}{z}.$$

In order to verify this, start with

$$(f_m)_*\phi = \sum_{j=1}^{m} \sigma_j^*(\phi(z)dz) = \sum_{k=-\infty}^{\infty} \sum_{j=1}^{m} a_k \sigma_j^*(z^k dz) = \sum_{k=-\infty}^{\infty} a_k (f_m)_*(z^k dz)$$

where $\sigma_1(w), ..., \sigma_m(w)$ are the m-*th root sections* of $w = f_m(z) = z^m$, defined by

$$\sigma_j(w) = e^{2\pi i j/m} \sigma_0(w)$$

where $\sigma_0(w) = w^{1/m}$ is the value of the complex m-th root whose argument is between

0 and $2\pi/m$. A direct calculation yields

$$\begin{aligned}
(f_m)_*(z^k dz) &= \sum_{j=1}^{m} \sigma_j^*(z^k dz) \\
&= \sum_{j=1}^{m} e^{2\pi ijk/m} w^{k/m} \left(\frac{1}{m} e^{2\pi ij/m} w^{1/m-1} \right) dw \\
&= \frac{1}{m} \left(\sum_{j=1}^{m} e^{2\pi ij(k+1)/m} \right) w^{(k+1-m)/m} dw \\
&= \begin{cases} z^{(k+1-m)/m} dz & \text{if } m|k+1, \\ 0 & \text{if } m|k+1. \end{cases}
\end{aligned}$$

This establishes the formula

$$(f_m)_*\phi = \sum_{k=-\infty}^{\infty} a_{m(k+1)-1} z^k dz.$$

Consequently,

$$\begin{aligned}
\left\| (f_m)_*^n \phi - a_{-1} \frac{dz}{z} \right\| &= \left\| \sum_{k=-\infty}^{\infty} a_{m^n(k+1)-1} z^k dz - a_{-1} \frac{dz}{z} \right\| \\
&= \sum_{k=-\infty, k\neq -1}^{\infty} |a_{m^n(k+1)-1}| R^{|k|} \\
&= \sum_{k=-\infty, k\neq -1}^{\infty} |a_{m^n(k+1)-1}| R^{|m^n(k+1)-1|} \frac{R^{|k|}}{R^{|m^n(k+1)-1|}} \\
&\leq \frac{R}{R^{m^n}} \sum_{k=-\infty, k\neq -1}^{\infty} |a_{m^n(k+1)-1}| R^{|m^n(k+1)-1|} \\
&\leq \frac{R}{R^{m^n}} \left\| \phi - a_{-1} \frac{dz}{z} \right\|.
\end{aligned}$$

As $n \to \infty$, this quantity converges to zero to order m. $\square$

Corollary 10.5.10. *For a rational function f*

$$\int_{-\infty}^{\infty} f(x)dx = \pi \lim_{n\to\infty} \mathcal{L}_m^n(f)(0)$$

provided that the integral is finite. In that case, convergence is of order m.

10.6 Implementation

In this section the implementation of the numerical scheme proposed in the previous sections is discussed. Assume that A and B are polynomials and let

$$I := \int_{-\infty}^{\infty} \frac{B(x)}{A(x)} dx. \tag{10.1}$$

The first issue under consideration is that the exact evaluation of the iterates of $\mathcal{L}_{m,p}^n(B/A)$ usually leads to extreme growth in the size of the coefficients. Therefore, while computing these iterates numerically, the coefficients are normalized after each iteration by keeping the denominator polynomial with leading coefficient 1.

Example 10.6.1. This continues Example 10.2.6 where

$$\int_{-\infty}^{\infty} \frac{dx}{x^2+4x+15} = \frac{\pi}{\sqrt{11}}$$

is approximated using $\mathcal{L}_{2,2}$. The first iterate is $\frac{32}{60x^2+112x+240}$. The next two Landen iterates are

$$\frac{19200}{57600x^2+40320x+77456}, \quad \frac{5186150400}{17845862400x^2+1601187840x+16614420736}.$$

Experiments show that the number of digits in the coefficients grows exponentially even if common factors are cancelled.

Fix $m \in \mathbb{N}$ and let $p = \deg(A)$. The normalization proceeds as follows: let

$$b_0 = (b_{0,0}, b_{0,1}, \ldots, b_{0,p-2}) \text{ and } a_0 = (a_{0,0}, a_{0,1}, \ldots, a_{0,p}) \tag{10.2}$$

be the coefficients of the initial rational function B/A. For $n \geq 1$, let

$$(b_n, a_n) = \frac{1}{a'_{n,0}}(b'_n, a'_n), \quad \text{where } (b'_n, a'_n) = \mathcal{L}_{m,p}(b_{n-1}, a_{n-1}). \tag{10.3}$$

Recall that the rational Landen transformations preserve the degree of the denominator. Hence, $a'_{n,0} \neq 0$ throughout. If the integral of B/A converges, then by Corollary 10.5.10 its value is given by $\pi \lim_{n\to\infty} b_{n,0}$.

Proposition 10.5.1 shows that, if the integral over B/A is finite, then a_n converges to the coefficients c_k of one of the $p+1$ candidates

$$(x-i)^k(x+i)^{p-k}, \quad 0 \leq k \leq p, \tag{10.4}$$

depending on the number k of roots of A with positive imaginary part. In particular, Corollary 10.5.2 shows that if all coefficients are real, then a_n will converge to

$$\left(\binom{p/2}{0}, 0, \binom{p/2}{1}, 0, \ldots, \binom{p/2}{p/2-1}, 0, \binom{p/2}{p/2}\right). \tag{10.5}$$

Conversely, if convergence to one of the candidates in (10.4) is observed, then the invariance of the integral under $\mathcal{L}_m$ shows that the initial integral must be finite. Thus the algorithm also detects the integrability of rational functions.

After each step, the implementation checks if the approximate relative error $|(b_{n,0} - b_{n-1,0})/b_{n,0}|$ is less than the precision goal. The distance of the coefficients a_n to their limiting values is also monitored. While computations may be made symbolically (provided that the initial coefficients are known exactly) it is generally sensible to work with a fixed precision throughout. For most integrands (compare Examples 10.2.6 and 10.4.1) this working precision need only be slightly larger, say 5 digits, than the precision goal. In case of almost singular integrands (compare Example 10.4.2) the working precision may need to be chosen somewhat higher. For the problems considered by the authors, a reasonable choice (currently used as a default in the Mathematica implementation mentioned below) seems to be 20 additional digits. The implementation of the Landen iteration method is given below in pseudo code.

Input: the coefficients (b_0, a_0) of the rational function B/A of degree p, the order m of the method, and the precision goal $\epsilon > 0$.

Output: an approximation (produced using Landen iterations of order m) to the integral of B/A over the real line with (approximate) relative error less than ϵ.

$n := 0$

repeat

$\quad n := n + 1$

$\quad (b'_n, a'_n) := \mathcal{L}_{m,p}(b_{n-1}, a_{n-1})$

$\quad (b_n, a_n) := \frac{1}{a'_{n,0}}(b'_n, a'_n)$

until $|(b_{n,0} - b_{n-1,0})/b_{n,0}| < \epsilon$ and $|(a_{n,j} - c_{k,j})/c_{k,j}| < \epsilon$

$\quad$ for all j and some $0 \leq k \leq p$

OUTPUT $\pi b_{n,0}$

The described method for integrating rational functions over the real line has been implemented in Mathematica and can be downloaded from the website

`http://www.math.tulane.edu/~vhm`

The Landen transformations can be either generated by the package, following the description in Section 10.2, or downloaded as well. The following examples demonstrate the basic usage of this package. Further examples can be obtained from the above website.

Example 10.6.2. Given a rational function f, its integral over the entire real line can be computed using the function `NLandenIntegrate`. For instance, to compute the integral of $1/(x^2 + 4x + 15)$ to a precision of 100 digits, input:

```
NLandenIntegrate[1/(x^2+4x+15), PrecisionGoal->100]
> 0.94722582509948293642963438181697406661998807...
```

By default the Landen transformation is chosen to be of order 2 (see Remark 10.3.3 for why this is desirable) but higher orders m may be used by setting `MethodOrder->m`. Further options exist to control the number of iterations, set the working precision manually, or to obtain the intermediate Landen iterates.

Example 10.6.3. Before using the function `NLandenIntegrate` demonstrated in the previous example the corresponding Landen transformation needs to be available. The command

```
GenerateLandenTransforms[10]
```

will generate the Landen transformations of order 2 for degrees up to 10. Note that on a modern desktop computer this will take less than half a second. After execution, the Landen transformations are directly available as follows, compare example 10.2.1:

```
LandenStep[{{b0}, {a0,a1,a2}}, 2]
> {{2a0b0+2a2b0}, {4a0a2, -2a0a1+2a1a2, a0^2-a1^2+2a0a2+a2^2}}
```

Again, higher orders than 2 can be generated using the option `MethodOrder`. Once generated, these Landen transformations may be stored to a file. Alternatively, pre-generated Landen transformations are available for download.

10.7 Conclusions

A numerical method for the integration of rational functions on the real line has been described. The method has order of convergence prescribed by the user. Its convergence and robustness have been analyzed. Examples illustrating speed of convergence as well as the flexibility of this method have been provided. A Mathematica package is available for the general public.

Future work will attempt to couple this method with Pade approximations of the integrand to produce a highly efficient numerical scheme for smooth integrable functions. The construction of a numerical scheme for the finite interval case requires the theory of Landen transformations on a half-line. This is an open question.

Chapter 11

Closed-form evaluation of integrals appearing in positronium decay

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[AMS09] *Closed-form evaluation of integrals appearing in positronium decay*
(with Tewodros Amdeberhan, Victor H. Moll)
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Abstract A theoretical prediction for the total width of the positronium decay in QED has been given by B. Kniehl et al. in the form of an expansion in Sommerfeld's fine-structure constant. The coefficients of this expansion are given in the form of two-dimensional definite integrals, with an integrand involving the polylogarithm function. We provide here an analytic expression for the one-loop contribution to this problem.

11.1 Introduction

The single-scale problems in multi-loop analytic calculations from quantum field theories yield interesting classes of integrals. Some examples have appeared in the recent work by B. Kniehl et al [KKV08a] and [KKV08b] dealing with the lifetime of one of the two ground states of the *positronium*. This is the electromagnetic bound state of the electron e^- and the positron e^+. The main result of [KKV08b] is a theoretical prediction for the total width of positronium decay in QED given by

$$\Gamma(\text{theory}) = \Gamma_0 \left[1 + \frac{A\alpha}{\pi} + \frac{1}{3}\alpha^2 \ln \alpha + B\left(\frac{\alpha}{\pi}\right)^2 - \frac{3\alpha^3 \ln^2 \alpha}{2\pi} + \frac{C\alpha^3 \ln \alpha}{\pi}\right], \tag{11.1}$$

where α is Sommerfeld's fine-structure constant. The leading order term $\Gamma_0 = 2(\pi^2 - 9)m\alpha^6/9\pi$, as well as the $O\left(\alpha^2 \ln \alpha\right)$ and $O\left(\alpha^3 \ln^2 \alpha\right)$ terms are in the literature (with A, B, C in numerical form only). The remarkable contribution of [KKV08b] is to provide the first analytic expression for the coefficients A and C in (11.1). An analogous expression for B still remains to be completed. The formulas for A and C consist of a formidable collection of terms involving special values of $\ln x$, the Riemann zeta function $\zeta(x)$, the polylogarithm $\mathrm{Li}_n(x)$ and the function

$$S_{n,p}(x) = \frac{(-1)^{n+p-1}}{(n-1)!\,p!}\int_0^1 \ln^{n-1} t\, \ln^p(1-tx)\,dt. \tag{11.2}$$

The explicit formulas can be found in [KKV08b].

The one-loop contribution to the width is given as

$$\Gamma_1 = \frac{m\alpha^7}{36\pi^2}\int_0^1 \frac{dx_1}{x_1}\frac{dx_2}{x_2}\frac{dx_3}{x_3}\delta(2 - x_1 - x_2 - x_3) \times \left[F(x_1, x_3) + \cdots\right], \tag{11.3}$$

where x_i, with $0 \le x_i \le 1$, is the normalized energy of the i-th photon and "..." represents F applied to each of the other five permutations of the variables. The evaluation of the integral (11.3) presents considerable analytic difficulties. After reparametrization, some terms in the function F involve integrals of the form

$$\begin{aligned} I_1(x_1, x_2) &= \int_0^1 \frac{\log[x_1 + (1-x_1)y^2]}{(1-x_1)x_2 - x_1(1-x_2)y^2}\,dy \\ I_2(x_1, x_2) &= \int_0^1 \frac{\log[x_1 + (1-x_1)y^2]}{x_1 x_2 - (1-x_1)(1-x_2)y^2}\,dy. \end{aligned} \tag{11.4}$$

The goal of this note is to present an analytic evaluation of the integrals (11.4). This evaluation includes elementary functions as well as the *dilogarithm function*

$$\mathrm{Li}_2(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2} = -\int_0^z \frac{\log(1-t)}{t}\,dt. \tag{11.5}$$

Remark 1.1. D. Zagier states in [Zag88] that 'the dilogarithm is one of the simplest non-elementary functions. It is also one of the strangest. ... Almost all of its appearances in mathematics, and almost all formulas relating to it, have something of the fantastical in them, as if this function alone among all others possessed a sense of humor.'

The following basic relations are due to Euler:

$$\begin{aligned}
\mathrm{Li}_2(z) + \mathrm{Li}_2(1-z) &= \frac{\pi^2}{6} - \log z\,\log(1-z), \\
\mathrm{Li}_2(z) + \mathrm{Li}_2(-z) &= \frac{1}{2}\mathrm{Li}_2(z^2), \\
\mathrm{Li}_2(z) + \mathrm{Li}_2(1/z) &= \frac{\pi^2}{3} - \frac{1}{2}\log^2(z) - i\pi\log z.
\end{aligned}$$

Information about dilogarithms can be found in [Lew81].

Notation. For $a \in \mathbb{R}$, we let $a^* := \dfrac{1-a}{1+a}$. Note that $(a^*)^* = a$, and $0 < a < 1$ if and only if $0 < a^* < 1$. For $a \in \mathbb{C}$, the condition $|a^*| \leq 1$ is equivalent to $\mathrm{Re}\, a > 0$. The functions

$$\ell(a,b) = \mathrm{Li}_2\left(\frac{1-a}{1-b}\right) \tag{11.6}$$

and

$$\ell_s(a,b) = \ell(a,b) - \ell(-a,b) - \ell(a,-b) + \ell(-a,-b) \tag{11.7}$$

are used to give an analytic expression for the integrals I_1 and I_2.

Theorem 11.1.1. *The positronium integrals are given by*

$$
\begin{aligned}
I_1\left(\frac{1}{1-t_1^2}, \frac{1}{1-t_2^2}\right) &= -\frac{(1-t_1^2)(1-t_2^2)}{2t_1t_2}\left(\log t_1^* \log\left((t_2/t_1^2)^*\right) - \ell_s(t_1, t_1^2/t_2)\right), \\
I_2\left(\frac{1}{1-t_1^2}, \frac{1}{1-t_2^2}\right) &= \frac{(1-t_1^2)(1-t_2^2)}{2t_1t_2}\left(\log t_1^* \log t_2^* - \ell_s(t_1, 1/t_2)\right).
\end{aligned}
$$

Remark 1.2. Kummer's formula for the dilogarithm [Lew81] is

$$
\begin{aligned}
\mathrm{Li}_2\left(\frac{x(1-y)^2}{y(1-x)^2}\right) &= \mathrm{Li}_2\left(\frac{x(1-y)}{x-1}\right) + \mathrm{Li}_2\left(\frac{1-y}{y(x-1)}\right) \\
&+ \mathrm{Li}_2\left(\frac{x(1-y)}{y(1-x)}\right) + \mathrm{Li}_2\left(\frac{1-y}{1-x}\right) + \frac{1}{2}\log^2 y.
\end{aligned}
$$

A change of variable gives the identity

$$\ell(a,b) + \ell(-a,b) + \ell(a,-b) + \ell(-a,-b) = \ell(a^2,b^2) - \frac{1}{2}\log^2(-b^*) \tag{11.8}$$

and shows that $\ell_s(a,b)$ may be expressed as a sum of three dilogarithms plus elementary functions.

11.2 Some logarithmic integrals

The hypergeometric function

$${}_pF_q\left(\begin{matrix} a_1,\, a_2, \cdots, a_p \\ b_1,\, b_2, \cdots, b_q \end{matrix}; z\right) := \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k \cdots (a_p)_k}{(b_1)_k (b_2)_k \cdots (b_q)_k} \frac{z^k}{k!}. \tag{11.1}$$

is now employed to establish the results in this section.

Lemma 11.2.1. *For $a \neq b$*

$$\int (1-ax)^{\lambda-1}(1-bx)^{\mu-1}dx = \frac{1}{\lambda}\frac{(1-ax)^{\lambda}(1-bx)^{\mu}}{b-a}\,{}_2F_1\left(\begin{matrix} 1, \lambda+\mu \\ \lambda+1 \end{matrix}; \frac{1-ax}{1-a/b}\right).$$

Proof. This is verified by differentiation both sides with respect to x. $\square$

Proposition 11.2.2. *For $a \neq b$*

$$\int_0^1 \frac{\log(1-ax)}{1-bx}\,dx = \frac{1}{b}\left[\mathrm{Li}_2\left(\frac{1}{1-a/b}\right) - \mathrm{Li}_2\left(\frac{1-a}{1-a/b}\right)\right.$$
$$\left. - \log(1-a)\log\left(\frac{1-b}{1-b/a}\right)\right],$$

$$\int_0^1 \frac{\log(1-a^2x^2)}{1-b^2x^2}\,dx = \frac{1}{2b}\left[\ell_s(a,a/b) + \log a^* \log((b/a)^*) - \log b^* \log(1-a^2)\right].$$

Proof. Lemma 11.2.1 yields

$$\int \frac{(1-ax)^{\lambda-1}}{1-bx}dx = \frac{1}{\lambda}\frac{(1-ax)^{\lambda}}{b-a}\,{}_2F_1\left(\begin{matrix}1,\lambda\\ \lambda+1\end{matrix};\frac{1-ax}{1-a/b}\right).$$

Observe that

$$\frac{d}{d\lambda}{}_2F_1\left(\begin{matrix}1,\lambda\\ \lambda+1\end{matrix};z\right) = \frac{z}{(1+\lambda)^2}\,{}_3F_2\left(\begin{matrix}2,\lambda+1,\lambda+1\\ \lambda+2,\,\lambda+2\end{matrix};z\right). \tag{11.2}$$

Differentiating with respect to λ leads to

$$\int \log(1-ax)\frac{(1-ax)^{\lambda-1}}{1-bx}\,dx =$$
$$\frac{1}{\lambda}\frac{(1-ax)^{\lambda}}{b-a}\left[\left(\log(1-ax)-\frac{1}{\lambda}\right){}_2F_1\left(\begin{matrix}1,\lambda\\ \lambda+1\end{matrix};\frac{1-ax}{1-a/b}\right)\right.$$
$$\left.+\frac{1-ax}{(1-a/b)(1+\lambda)^2}\,{}_3F_2\left(\begin{matrix}2,\lambda+1,\lambda+1\\ \lambda+2,\,\lambda+2\end{matrix};\frac{1-ax}{1-a/b}\right)\right].$$

Now set $\lambda=1$ and use $\mathrm{Li}_1(z) = -\log(1-z)$, as well as

$${}_3F_2\left(\begin{matrix}2,\,2,\,2\\ 3,\,3\end{matrix};z\right) = -\frac{4}{z^2}\left[\log(1-z)+\mathrm{Li}_2(z)\right] \tag{11.3}$$

to establish the first claim. The factorization $(1-a^2x^2) = (1-ax)(1+ax)$ and the partial fraction decomposition

$$\frac{2}{1-b^2x^2} = \frac{1}{1-bx} + \frac{1}{1+bx} \tag{11.4}$$

give the second evaluation. □

11.3 A trigonometric integral

The results in Section 11.2 provide the value of an interesting trigonometric integral in terms of Legendre's χ_2 function

$$\chi_2(a) := \frac{1}{2}\left(\mathrm{Li}_2(a) - \mathrm{Li}_2(-a)\right). \tag{11.1}$$

Proposition 11.3.1. *For $a \in \mathbb{R}$*

$$\int_b^\infty \frac{\tan^{-1}(ax)}{1+x^2}\,dx = \chi_2(a) + \frac{1}{2}\log a \log a^* + \frac{1}{4}\ell_s(a, i/b). \tag{11.2}$$

Proof. Observe that

$$\begin{aligned} \frac{d}{da}\int_b^\infty \frac{\tan^{-1}(ax)\,dx}{1+x^2} &= \int_b^\infty \frac{x\,dx}{(1+a^2x^2)(1+x^2)} \\ &= \frac{1}{2(1-a^2)}\left(\log(1+a^2b^2) - 2\log a - \log(1+b^2)\right). \end{aligned}$$

The original integral is recovered via

$$\int_0^a \frac{ds}{1-s^2} = \frac{1}{2}\log\left(\frac{1+a}{1-a}\right) = -\frac{1}{2}\log a^*, \tag{11.3}$$

as well as

$$\int_0^a \frac{2\log s\, ds}{1-s^2} = \mathrm{Li}_2(1-a) - \mathrm{Li}_2(1) + \mathrm{Li}_2(-a) + \log a\, \log(1+a). \tag{11.4}$$

The last term to evaluate

$$\int_0^a \frac{\log(1+s^2b^2)}{1-s^2}\, ds = a \int_0^1 \frac{\log(1+a^2b^2x^2)}{1-a^2x^2}\, dx, \tag{11.5}$$

is given by Proposition 11.2.2 as

$$\frac{1}{2}\left[\ell_s(iab, ib) + \log((iab)^*)\log(-(ib)^*) - \log(a^*)\log(1+a^2b^2)\right]. \tag{11.6}$$

The result now follows from Euler's transformations for the dilogarithm given after Remark 1.1. □

Letting $b \to 0$ produces the integral over the half-line.

Corollary 11.3.2. *The evaluation*

$$\int_0^\infty \frac{\tan^{-1}(ax)\, dx}{1+x^2} = \chi_2(a) + \frac{1}{2}\log a \log(a^*). \tag{11.7}$$

holds.

11.4 Application to the positronium decay integrals

For the convenience of the reader we reproduce Theorem 11.1.1:

Theorem 11.4.1. *The positronium integrals are given by*

$$\begin{aligned} I_1\left(\frac{1}{1-t_1^2},\frac{1}{1-t_2^2}\right) &= -\frac{(1-t_1^2)(1-t_2^2)}{2t_1t_2}\left(\log t_1^*\,\log\left((t_2/t_1^2)^*\right)-\ell_s(t_1,t_1^2/t_2)\right), \\ I_2\left(\frac{1}{1-t_1^2},\frac{1}{1-t_2^2}\right) &= \frac{(1-t_1^2)(1-t_2^2)}{2t_1t_2}\left(\log t_1^*\,\log t_2^*-\ell_s(t_1,1/t_2)\right). \end{aligned}$$

Proof. The integral $I_1(x_1,x_2)$ is written as

$$\frac{-t_1^2}{(1-t_1^2)(1-t_2^2)}I_1\left(\frac{1}{1-t_1^2},\frac{1}{1-t_2^2}\right)=\int_0^1\log\left(\frac{1-t_1^2y^2}{1-t_1^2}\right)\frac{dy}{1-(t_2/t_1)^2y^2}. \tag{11.1}$$

Proposition 11.2.2 yields

$$\begin{aligned} \int_0^1\log\left(\frac{1-t_1^2y^2}{1-t_1^2}\right)\frac{dy}{1-(t_2/t_1)^2y^2} &= \int_0^1\frac{\log(1-t_1^2y^2)}{1-(t_2/t_1)^2y^2}\,dy-\int_0^1\frac{\log(1-t_1^2)}{1-(t_2/t_1)^2y^2}\,dy \\ &= \frac{t_1}{2t_2}\left[\log t_1^*\log((t_2/t_1^2)^*)-\ell_s(t_1,t_1^2/t_2)\right]. \end{aligned}$$

The second positronium integral is evaluated analogously. $\square$

The following special case is recorded.

Corollary 11.4.2. *Assume* $0<a<1$. *Then*

$$\int_0^1\frac{\log(a+(1-a)x^2)}{1-x^2}\,dx=-\arctan^2\left(\sqrt{\frac{1-a}{a}}\right). \tag{11.2}$$

Proof. Let $a=1/(1-t^2)$. Then

$$\begin{aligned} \int_0^1\frac{\log(a+(1-a)x^2)}{1-x^2}\,dx &= a(1-a)I_1(a,a) \\ &= \frac{1}{2}\left[\log t^*\log((1/t)^*)-\ell_s(t,t)\right]. \end{aligned}$$

It follows from Remark 1.1 that

$$\ell_s(t,t) = \frac{\pi^2}{3} - \mathrm{Li}_2\left(\frac{1-t}{1+t}\right) - \mathrm{Li}_2\left(\frac{1+t}{1-t}\right) = \frac{1}{2}\log^2 t^* + i\pi \log t^*. \tag{11.3}$$

Thus

$$\int_0^1 \frac{\log(a+(1-a)x^2)}{1-x^2}\,dx = \left(\frac{1}{2}\log t^*\right)^2 \tag{11.4}$$

and this is (11.2). □

Chapter 12

Wallis-Ramanujan-Schur-Feynman

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[AEMS10] *Wallis-Ramanujan-Schur-Feynman*
(with Tewodros Amdeberhan, Olivier Espinosa, Victor H. Moll)
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Abstract One of the earliest examples of analytic representations for π is given by an infinite product provided by Wallis in 1655. The modern literature often presents this evaluation based on the integral formula

$$\frac{2}{\pi}\int_0^\infty \frac{dx}{(x^2+1)^{n+1}} = \frac{1}{2^{2n}}\binom{2n}{n}.$$

In trying to understand the behavior of this integral when the integrand is replaced by the inverse of a product of distinct quadratic factors, the authors encounter relations to some formulas of Ramanujan, expressions involving Schur functions, and Matsubara sums that have appeared in the context of Feynman diagrams.

12.1 Wallis' infinite product for π

Among the earliest analytic expressions for π one finds two infinite products: the first one given by Vieta [Vie70] in 1593,

$$\frac{2}{\pi} = \sqrt{\frac{1}{2}}\sqrt{\frac{1}{2}+\frac{1}{2}\sqrt{\frac{1}{2}}}\sqrt{\frac{1}{2}+\frac{1}{2}\sqrt{\frac{1}{2}+\frac{1}{2}\sqrt{\frac{1}{2}}}}\cdots,$$

and the second by Wallis [Wal86] in 1655,

$$\frac{2}{\pi} = \frac{1\cdot 3}{2\cdot 2}\cdot\frac{3\cdot 5}{4\cdot 4}\cdot\frac{5\cdot 7}{6\cdot 6}\cdot\frac{7\cdot 9}{8\cdot 8}\cdots. \tag{12.1}$$

In this journal, T. Osler [Osl99] has presented the remarkable formula

$$\frac{2}{\pi} = \prod_{n=1}^{p}\sqrt{\frac{1}{2}+\frac{1}{2}\sqrt{\frac{1}{2}+\sqrt{\frac{1}{2}+\cdots+\frac{1}{2}\sqrt{\frac{1}{2}}}}}\prod_{n=1}^{\infty}\frac{2^{p+1}n-1}{2^{p+1}n}\cdot\frac{2^{p+1}n+1}{2^{p+1}n},$$

where the nth term in the first product has n radical signs. This equation becomes Wallis' product when $p=0$ and Vieta's formula as $p\to\infty$. It is surprising that such a connection between the two products was not discovered earlier.

The collection [BBB97] contains both original papers of Vieta and Wallis as well as other fundamental papers in the history of π. Indeed, there are many good historical sources on π. The text by P. Eymard and J. P. Lafon [EL04] is an excellent place to start.

Wallis' formula (12.1) is equivalent to

$$W_n := \prod_{k=1}^{n}\frac{(2k)\cdot(2k)}{(2k-1)\cdot(2k+1)} = \frac{2^{4n}}{\binom{2n}{n}\binom{2n+1}{n}(n+1)} \to \frac{\pi}{2} \tag{12.2}$$

as $n \to \infty$. This may be established using Stirling's approximation

$$m! \sim \sqrt{2\pi m}\left(\frac{m}{e}\right)^m.$$

Alternatively, there are many elementary proofs of (12.2) in the literature. Among them, [Was07] and [LD09] have recently appeared in this journal.

Section 12.3 presents a proof of (12.2) based on the evaluation of the rational integral

$$G_n := \frac{2}{\pi}\int_0^\infty \frac{dx}{(x^2+1)^n}. \tag{12.3}$$

This integral is discussed in the next section. The motivation to generalize (12.3) has produced interesting links to symmetric functions from combinatorics and to one-loop Feynman diagrams from particle physics. The goal of this work is to present these connections.

12.2 A rational integral and its trigonometric version

The method of partial fractions reduces the integration of a rational function to an algebraic problem: the factorization of its denominator. The integral (12.3) corresponds to the presence of purely imaginary poles. See [BM04] for a treatment of these ideas.

A recurrence for G_n is obtained by writing $1 = (x^2+1) - x^2$ for the numerator of (12.3) and integrating by parts. The result is

$$G_{n+1} = \frac{2n-1}{2n}G_n. \tag{12.4}$$

Since $G_1 = 1$ it follows that

$$G_{n+1} = \frac{1}{2^{2n}} \binom{2n}{n}. \tag{12.5}$$

The choice of a new variable is one of the fundamental tools in the evaluation of definite integrals. The new variable, if carefully chosen, usually simplifies the problem or opens up unsuspected possibilities. Trigonometric changes of variables are considered *elementary* because these functions appear early in the scientific training. Unfortunately, this hides the fact that this change of variables introduces a *transcendental function* with a multivalued inverse. One has to proceed with care.

The change of variables $x = \tan\theta$ in the definition (12.3) of G_n gives

$$G_{n+1} = \frac{2}{\pi} \int_0^{\pi/2} (\cos\theta)^{2n} \, d\theta.$$

In this context, the recurrence (12.4) is obtained by writing

$$(\cos\theta)^{2n} = (\cos\theta)^{2n-2} + \frac{\sin\theta}{2n-1} \frac{d}{d\theta} (\cos\theta)^{2n-1}$$

and then integrating by parts. Yet another recurrence for G_n is obtained by a double-angle substitution yielding

$$G_{n+1} = \frac{2}{\pi} \int_0^{\pi/2} \left(\frac{1+\cos 2\theta}{2} \right)^n d\theta,$$

and a binomial expansion (observe that the odd powers of cosine integrate to zero). It follows that

$$G_{n+1} = 2^{-n} \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{2k} G_{k+1}.$$

Thus, (12.5) is equivalent to proving the finite sum identity

$$\sum_{k=0}^{\lfloor n/2 \rfloor} 2^{-2k} \binom{n}{2k} \binom{2k}{k} = 2^{-n} \binom{2n}{n}. \tag{12.6}$$

There are many possible ways to prove this identity. For instance, it is a perfect candidate for the truly 21st-century WZ method [PWZ96] that provides automatic proofs; or, as pointed out by M. Hirschhorn in [Hir02], it is a disguised form of the Chu-Vandermonde identity

$$\sum_{k\geq 0}\binom{x}{k}\binom{y}{k}=\binom{x+y}{x} \tag{12.7}$$

(which was discovered first in 1303 by Zhu Shijie). Namely, upon employing Legendre's duplication formula for the gamma function

$$\Gamma(\tfrac{1}{2})\Gamma(2z+1)=2^{2z}\Gamma(z+1)\Gamma(z+\tfrac{1}{2}),$$

the identity (12.6) can be rewritten as

$$\sum_{k\geq 0}\binom{\frac{n}{2}}{k}\binom{\frac{n}{2}-\frac{1}{2}}{k}=\binom{n-\frac{1}{2}}{\frac{n}{2}-\frac{1}{2}}.$$

This is a special case of (12.7). Another, particularly nice and direct, proof of (12.6), as kindly pointed out by one of the referees, is obtained from looking at the constant coefficient of

$$\left(\frac{x}{2}+\frac{x^{-1}}{2}+1\right)^{n}=2^{-n}\left(x^{1/2}+x^{-1/2}\right)^{2n}.$$

Remark 12.2.1. The idea of double-angle reduction lies at the heart of the *rational Landen transformations*. These are polynomial maps on the coefficient of the integral of a rational function that preserve its value. See [MM08a] for a survey on Landen transformations and open questions.

12.3 A squeezing method

In this section we employ the explicit expression for G_n given in (12.5) to establish Wallis' formula (12.1). This approach is also contained in Stewart's calculus text book [Ste07] in the form of several guided exercises (45, 46, and 68 of Section 7.1). The proof is based on analyzing the integrals

$$I_n := \int_0^{\pi/2} (\sin x)^n \, dx.$$

The formula

$$I_{2n} = \int_0^{\pi/2} (\sin x)^{2n} \, dx = \frac{(2n-1)!!}{(2n)!!} \frac{\pi}{2}$$

follows from (12.5) by symmetry. Its companion integral

$$I_{2n+1} = \int_0^{\pi/2} (\sin x)^{2n+1} \, dx = \frac{(2n)!!}{(2n+1)!!}$$

is of the same flavor. Here $n!! = n(n-2)(n-4)\cdots\{1 \text{ or } 2\}$ denotes the double factorial. The ratio of these two integrals gives

$$W_n I_{2n}/I_{2n+1} = \frac{\pi}{2},$$

where W_n is defined by (12.2). The convergence of W_n to $\pi/2$ now follows from the inequalities $1 \leq I_{2n}/I_{2n+1} \leq 1 + 1/(2n)$. The first of these inequalities is equivalent to $I_{2n+1} \leq I_{2n}$, which holds because $(\sin x)^{2n+1} \leq (\sin x)^{2n}$. The second is equivalent to

$$2n \int_0^{\pi/2} (\sin x)^{2n} \, dx \leq (2n+1) \int_0^{\pi/2} (\sin x)^{2n+1} \, dx,$$

which follows directly from the bound $I_{2n} \leq I_{2n-1}$ and the recurrence $(2n+1)I_{2n+1} = 2nI_{2n-1}$. Alternatively, the second inequality can be proven by observing that the function

$$f(s) = s \int_0^{\pi/2} (\sin x)^s \, dx$$

is increasing. This may be seen from the change of variables $t = \sin x$ and a series expansion of the new integrand yielding

$$f'(s) = \sum_{k=0}^{\infty} \frac{1}{2^{2k}} \binom{2k}{k} \frac{2k+1}{(2k+s+1)^2} > 0. \tag{12.8}$$

Remark 12.3.1. Comparing the series (12.8) at $s = 0$ with the limit

$$f'(0) = \lim_{s \to 0} \frac{f(s)}{s} = \lim_{s \to 0} \int_0^{\pi/2} \sin^s x \, dx = \frac{\pi}{2}$$

immediately proves

$$\sum_{k=0}^{\infty} \binom{2k}{k} \frac{2^{-2k}}{2k+1} = \frac{\pi}{2}.$$

This value may also be obtained by letting $x = \frac{1}{2}$ in the series

$$\sum_{k=0}^{\infty} \binom{2k}{k} \frac{x^{2k}}{2k+1} = \frac{\text{arcsin} 2x}{2x}.$$

The reader will find in [Leh85] a host of other interesting series that involve the central binomial coefficients.

12.4 An example of Ramanujan and a generalization

A natural generalization of Wallis' integral (12.3) is given by

$$G_n(\boldsymbol{q}) = \frac{2}{\pi} \int_0^{\infty} \prod_{k=1}^{n} \frac{1}{x^2 + q_k^2} \, dx, \tag{12.9}$$

where $\boldsymbol{q} = (q_1, q_2, \ldots, q_n)$ with $q_k \in \mathbb{C}$. This notation will be employed throughout. Similarly, $\boldsymbol{q}^\alpha$ is used to denote $(q_1^\alpha, q_2^\alpha, \ldots, q_n^\alpha)$. As the value of the integral (12.9) is fixed under a change of sign of the parameters q_k, it is assumed that Re $q_k > 0$. Note that the integral $G_n(\boldsymbol{q})$ is a symmetric function of $\boldsymbol{q}$ that reduces to G_n in the special case $q_1 = \cdots = q_n = 1$.

The special case $n = 4$ appears as Entry 13, Chapter 13 of volume 2 of B. Berndt's *Ramanujan's Notebooks* [Ber89], in the form[1]:

Example 12.4.1. Let q_1, q_2, q_3, and q_4 be positive real numbers. Then

$$\frac{2}{\pi}\int_0^\infty \frac{dx}{(x^2+q_1^2)(x^2+q_2^2)(x^2+q_3^2)(x^2+q_4^2)} = \frac{(q_1+q_2+q_3+q_4)^3 - (q_1^3+q_2^3+q_3^3+q_4^3)}{3q_1q_2q_3q_4(q_1+q_2)(q_2+q_3)(q_1+q_3)(q_1+q_4)(q_2+q_4)(q_3+q_4)}.$$

Using partial fractions the following general formula for $G_n(\boldsymbol{q})$ is obtained. In the next section a representation in terms of Schur functions is presented.

Lemma 12.4.2. *Let* $\boldsymbol{q} = (q_1, \ldots, q_n)$ *be distinct and* Re $q_k > 0$. *Then*

$$G_n(\boldsymbol{q}) = \sum_{k=1}^n \frac{1}{q_k} \prod_{\substack{j=1 \\ j\neq k}}^n \frac{1}{q_j^2 - q_k^2}. \tag{12.10}$$

Proof. Observe first that if $b_1, b_2, \ldots, b_n$ are distinct then

$$\prod_{k=1}^n \frac{1}{y+b_k} = \sum_{k=1}^n \frac{1}{y+b_k} \prod_{\substack{j=1 \\ j\neq k}}^n \frac{1}{b_j - b_k}. \tag{12.11}$$

Replacing y by x^2 and b_k by q_k^2 and using the elementary integral

$$\frac{2}{\pi}\int_0^\infty \frac{dx}{x^2+q^2} = \frac{1}{q}$$

[1] A minor correction from [Ber89].

produces the desired evaluation of $G_n(\boldsymbol{q})$. $\square$

Remark 12.4.3. $G_n(\boldsymbol{q})$, as defined by (12.9), is a symmetric function in the q_i's which remains finite if two of these parameters coincide. Therefore, the factors $q_j - q_k$ in the denominator of the right-hand side of (12.10) cancel out. This may be checked directly by combining the summands corresponding to j and k. Alternatively, note that the right-hand side of (12.10) is symmetric while the critical factors $q_j - q_k$ in the denominator combine to form the antisymmetric Vandermonde determinant. Accordingly, they have to cancel.

Example 12.4.4. The identities

$$\frac{2}{\pi}\int_0^\infty \prod_{j=1}^{n+1} \frac{1}{x^2+j^2}\,dx = \frac{1}{(2n+1)n!(n+1)!},$$
$$\frac{2}{\pi}\int_0^\infty \prod_{j=1}^{n+1} \frac{1}{x^2+(2j-1)^2}\,dx = \frac{1}{2^{2n}(2n+1)(n!)^2},$$
$$\frac{2}{\pi}\int_0^\infty \prod_{j=1}^{n} \frac{1}{x^2+1/j^2}\,dx = \frac{2A(2n-1,n-1)}{\binom{2n}{n}}$$

may be deduced inductively from Lemma 12.4.2. Here, $A(n,k)$ are the Eulerian numbers which count the number of permutations of n objects with exactly k descents. Recall that a permutation σ of the n letters $1, 2, \ldots, n$, here written as $\sigma(1)\,\sigma(2)\,\ldots\,\sigma(n)$, has a descent at position k if $\sigma(k) > \sigma(k+1)$. For instance, $A(3,1) = 4$ because there are 4 permutations of $1, 2, 3$, namely $1\,3\,2$, $2\,1\,3$, $2\,3\,1$, and $3\,1\,2$, which have exactly one descent.

The problem of finding an explicit formula for the numerator appearing on the right-hand side of (12.10) when put on the lowest common denominator is discussed in the next section.

12.5 Representation in terms of Schur functions

The expression for $G_n(\boldsymbol{q})$ developed in this section is given in terms of *Schur functions*. The reader is referred to [Bre99] for a motivated introduction to these functions in the context of *alternating sign matrices* and to [Sag01] for their role in the representation theory of the symmetric group. Among the many equivalent definitions for Schur functions, we now recall their definition in terms of quotients of alternants. Using this approach, we are able to associate a Schur function not only to a partition but more generally to an arbitrary vector.

Here, a vector $\mu = (\mu_1, \mu_2, \ldots)$ means a finite sequence of real numbers. μ is further called a partition (of m) if $\mu_1 \geqslant \mu_2 \geqslant \cdots$ and all the parts μ_j are positive integers (summing up to m). Write $\mathbf{1}^n$ for the partition with n ones, and denote by $\lambda(n)$ the partition

$$\lambda(n) = (n-1, n-2, \ldots, 1).$$

Vectors and partitions may be added componentwise. In case they are of different length, the shorter one is padded with zeroes. For instance, one has $\lambda(n+1) = \lambda(n)+\mathbf{1}^n$. Likewise, vectors and partitions may be multiplied by scalars. In particular, $a \cdot \mathbf{1}^n$ is the partition with n a's.

Fix n and consider $\boldsymbol{q} = (q_1, q_2, \ldots, q_n)$. Let $\mu = (\mu_1, \mu_2, \ldots)$ be a vector of length at most n. The corresponding alternant a_μ is defined as the determinant

$$a_\mu(\boldsymbol{q}) = \left| q_i^{\mu_j} \right|_{1 \leqslant i,j \leqslant n}.$$

Again, μ is padded with zeroes if necessary. Note that the alternant $a_{\lambda(n)}$ is the classical Vandermonde determinant

$$a_{\lambda(n)}(\boldsymbol{q}) = \left| q_i^{n-j} \right|_{1 \leqslant i,j \leqslant n} = \prod_{1 \leqslant i < j \leqslant n} (q_i - q_j).$$

The Schur function s_μ associated with the vector μ can now be defined as

$$s_\mu(\boldsymbol{q}) = \frac{a_{\mu+\lambda(n)}(\boldsymbol{q})}{a_{\lambda(n)}(\boldsymbol{q})}.$$

If μ is a partition with integer entries this is a symmetric polynomial. Indeed, as μ ranges over the partitions of m of length at most n, the Schur functions $s_\mu(\boldsymbol{q})$ form a basis for the homogeneous symmetric polynomials in $\boldsymbol{q}$ of degree m.

The Schur functions include as special cases the *elementary symmetric functions* e_k and the *complete homogeneous symmetric functions* h_k. Namely, $e_k(\boldsymbol{q}) = s_{\mathbf{1}^k}(\boldsymbol{q})$ and $h_k(\boldsymbol{q}) = s_{(k)}(\boldsymbol{q})$.

The next result expresses the integral $G_n(\boldsymbol{q})$ defined in (12.9) as a quotient of Schur functions.

Theorem 12.5.1. *Let* $\boldsymbol{q} = (q_1, \ldots, q_n)$ *and* $\operatorname{Re} q_k > 0$. *Then*

$$G_n(\boldsymbol{q}) = \frac{s_{\lambda(n-1)}(\boldsymbol{q})}{s_{\lambda(n+1)}(\boldsymbol{q})} = \frac{s_{\lambda(n-1)}(\boldsymbol{q})}{e_n(\boldsymbol{q}) s_{\lambda(n)}(\boldsymbol{q})}. \tag{12.12}$$

Proof. The equality $e_n(\boldsymbol{q}) s_{\lambda(n)}(\boldsymbol{q}) = s_{\lambda(n+1)}(\boldsymbol{q})$ amounts to the identity

$$q_1 q_2 \cdots q_n \left| q_i^{2n-2j} \right|_{i,j} = \left| q_i^{2n-2j+1} \right|_{i,j},$$

which follows directly by inserting the factor q_i into row i of the matrix.

From the previous definition of Schur functions, the right-hand side of (12.12) becomes

$$\frac{s_{\lambda(n-1)}(\boldsymbol{q})}{e_n(\boldsymbol{q})\, s_{\lambda(n)}(\boldsymbol{q})} = \frac{a_{\lambda(n-1)+\lambda(n)}(\boldsymbol{q})}{e_n(\boldsymbol{q}) a_{2\lambda(n)}(\boldsymbol{q})}.$$

Observe that $a_{2\lambda(n)}(\boldsymbol{q}) = |q_i^{2n-2j}|_{i,j} = a_{\lambda(n)}(\boldsymbol{q}^2)$ is simply the Vandermonde determinant with q_i replaced by q_i^2. Next, expand the determinant $a_{\lambda(n-1)+\lambda(n)}$ by the last column (which consists of 1's only) to find

$$a_{\lambda(n-1)+\lambda(n)}(\boldsymbol{q}) = e_n(\boldsymbol{q}) \sum_{k=1}^{n} \frac{(-1)^{n-k}}{q_k} a_{\lambda(n-1)}(q_1^2, q_2^2, \dots, q_{k-1}^2, q_{k+1}^2, \dots, q_n^2).$$

Therefore

$$\frac{a_{\lambda(n-1)+\lambda(n)}(\boldsymbol{q})}{e_n(\boldsymbol{q})\, a_{2\lambda(n)}(\boldsymbol{q})} = \sum_{k=1}^{n} \frac{(-1)^{n-k}}{q_k} \prod_{\substack{i<j \\ i,j\neq k}} (q_i^2 - q_j^2) \Big/ \prod_{i<j} (q_i^2 - q_j^2). \tag{12.13}$$

Observe that the only terms that do not cancel in the quotient above are those for which $i = k$ or $j = k$. The change of sign required to transform the factors $q_k^2 - q_j^2$ to $q_j^2 - q_k^2$ eliminates the factor $(-1)^{n-k}$. The expression on the right-hand side of (12.13) is precisely the value (12.10) of the integral $G_n(\boldsymbol{q})$ produced by partial fractions. □

The next example illustrates Theorem 12.5.1 with the principal specialization of the parameters $\boldsymbol{q}$.

Example 12.5.2. The special case $q_k = q^k$ produces the evaluation

$$\frac{2}{\pi} \int_0^\infty \prod_{k=1}^{n} \frac{1}{x^2 + q^{2k}} = \frac{1}{q^{n^2}} \prod_{j=1}^{n-1} \frac{1 - q^{2j-1}}{1 - q^{2j}}. \tag{12.14}$$

This can be obtained inductively from Lemma 12.4.2 but may also be derived from Theorem 12.5.1 in combination with the evaluation (12.15) of the principal specialization of Schur functions as in Theorem 7.21.2 of [Sta99].

Taking the limit $q \to 1$ in (12.14) reproduces formula (12.5) for G_n. In other words, (12.14) is a q-analog [GR90] of (12.5). Similarly,

$$\frac{\pi_q}{1+q} = q^{1/4} \prod_{n=1}^{\infty} \frac{1 - q^{2n}}{1 - q^{2n-1}} \frac{1 - q^{2n}}{1 - q^{2n+1}}$$

is a useful q-analog of Wallis' formula (12.2) which naturally appears in [Jr.00], where Gosper studies q-analogs of trigonometric functions (in fact, Gosper arrives at the above expression as a definition for π_q while q-generalizing the reflection formula $\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}$).

The proof of Theorem 12.5.1 extends to the following more general result.

Lemma 12.5.3.

$$\sum_{k=1}^{n} \frac{1}{q_k^{\alpha-\beta}} \prod_{\substack{j=1\\ j\neq k}}^{n} \frac{1}{q_j^\alpha - q_k^\alpha} = \frac{s_\lambda(\boldsymbol{q})}{s_\mu(\boldsymbol{q})},$$

where

$$\begin{aligned} \lambda &= (\alpha-1)\cdot\lambda(n) - \beta\cdot \mathbf{1}^{n-1}, \\ \mu &= (\alpha-1)\cdot\lambda(n+1) - (\beta-1)\cdot\mathbf{1}^{n}. \end{aligned}$$

As a consequence, one obtains the following integral evaluation which generalizes the evaluation of $G_n(\boldsymbol{q})$ given in Theorem 12.5.1.

Theorem 12.5.4. *Let* $\boldsymbol{q} = (q_1, \ldots, q_n)$ *and* $\operatorname{Re} q_k > 0$*. Further, let* α *and* β *be given such that* $\alpha > 0$*,* $0 < \beta < \alpha n$*, and* β *is not an integer multiple of* α*. Then*

$$G_{n,\alpha,\beta}(\boldsymbol{q}) := \frac{\sin(\pi\beta/\alpha)}{\pi/\alpha} \int_0^\infty \frac{x^{\beta-1}}{\prod_{k=1}^n (x^\alpha + q_k^\alpha)}\, dx = \frac{s_\lambda(\boldsymbol{q})}{s_\mu(\boldsymbol{q})},$$

where λ *and* μ *are as in Lemma 12.5.3.*

Proof. Upon writing $\beta = b\alpha + \beta_1$ for $b < n$ a positive integer and $0 < \beta_1 < \alpha$, the assertion follows from the partial fraction decomposition

$$\frac{x^{b\alpha}}{\prod_{k=1}^n (x^\alpha + q_k^\alpha)} = (-1)^b \sum_{k=1}^{n} \frac{q_k^{b\alpha}}{x^\alpha + q_k^\alpha} \prod_{j\neq k} \frac{1}{q_j^\alpha - q_k^\alpha},$$

the integral evaluation

$$\int_0^\infty \frac{x^{\beta_1-1}dx}{x^\alpha+q^\alpha} = \frac{1}{q^{\alpha-\beta_1}} \frac{\pi/\alpha}{\sin(\pi\beta_1/\alpha)},$$

and Lemma 12.5.3. □

12.6 Schur functions in terms of SSYT

The Schur function $s_\lambda(\boldsymbol{q})$ associated to a partition λ also admits a representation in terms of *semi-standard Young tableaux* (SSYT). The reader will find information about this topic in [Bre99]. Given a partition $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_m)$, the Young diagram of shape λ is an array of boxes, arranged in left-justified rows, consisting of λ_1 boxes in the first row, λ_2 in the second row, and so on, ending with λ_m boxes in the mth row. A SSYT of shape λ is a Young diagram of shape λ in which the boxes have been filled with positive integers. These integers are restricted to be weakly increasing across rows (repetitions are allowed) and strictly increasing down columns. From this point of view, the Schur function $s_\lambda(\boldsymbol{q}) = s_\lambda(q_1, \dots, q_n)$ can be defined as

$$s_\lambda(\boldsymbol{q}) = \sum_T \boldsymbol{q}^T,$$

where the sum is over all SSYT of shape λ with entries from $\{1, 2, \dots, n\}$. The symbol $\boldsymbol{q}^T$ is a monomial in the variables q_j in which the exponent of q_j is the number of appearances of j in T. For example, the array shown in Figure 12.1 is a tableau T for the partition $(6, 4, 3, 3)$. The corresponding monomial $\boldsymbol{q}^T$ is given by $q_1q_2^3q_3q_4^3q_5^4q_6^2q_7q_8$.

The number $N_n(\lambda)$ of SSYT of shape λ with entries from $\{1, 2, \dots, n\}$ can be

1	2	2	4	5	5
2	3	4	5		
4	6	6			
5	7	8			

Figure 12.1: A tableau T for the partition $(6,4,3,3)$.

obtained by letting $q \to 1$ in the formula

$$s_\lambda(1, q, q^2, \dots, q^{n-1}) = \prod_{1 \leq i < j \leq n} \frac{q^{\lambda_i+n-i} - q^{\lambda_j+n-j}}{q^{j-1} - q^{i-1}} \tag{12.15}$$

(see page 375 of [Sta99]). This yields

$$N_n(\lambda) = \prod_{1 \leq i < j \leq n} \frac{\lambda_i - \lambda_j + j - i}{j - i}. \tag{12.16}$$

The evaluation (12.5) of Wallis' integral (12.3) may be recovered from here as

$$G_{n+1} = \frac{s_{\lambda(n)}(\mathbf{1}^{n+1})}{s_{\lambda(n+2)}(\mathbf{1}^{n+1})} = \frac{N_{n+1}(\lambda(n))}{N_{n+1}(\lambda(n+2))} = \frac{1}{2^{2n}}\binom{2n}{n}.$$

12.7 A counting problem

The k-central binomial coefficients $c(n,k)$, defined by the generating function

$$(1 - k^2 x)^{-1/k} = \sum_{n \geq 0} c(n,k) x^n,$$

are given by

$$c(n,k) = \frac{k^n}{n!} \prod_{m=1}^{n-1} (1 + km).$$

For $k = 2$ these coefficients reduce to the central binomial coefficients $\binom{2n}{n}$. The numbers $c(n,k)$ are integers in general and their divisibility properties have been studied in [SMA09]. In particular, the authors establish that the k-central binomial coefficients are always divisible by k and characterize their p-adic valuations.

The next result attempts an (admittedly somewhat contrived) interpretation of what the numbers $-c(n,-k)$ count.

Corollary 12.7.1. *Let λ and μ be the partitions given by*

$$\begin{aligned} \lambda &= (k-1)\cdot\lambda(n) - \mathbf{1}^{n-1}, \\ \mu &= (k-1)\cdot\lambda(n+1). \end{aligned}$$

Then the integer $-c(n,-k)$ enumerates the ratio between the total number of SSYT of shapes λ and μ with entries from $\{1,2,\ldots,n\}$ times the factor k^{2n-1}/n.

Proof. By Theorem 12.5.4,

$$\frac{N_n(\lambda)}{N_n(\mu)} = \frac{s_\lambda(\mathbf{1}^n)}{s_\mu(\mathbf{1}^n)} = G_{n,k,1}(\mathbf{1}^n) = \frac{\sin(\pi/k)}{\pi/k}\int_0^\infty \frac{1}{(x^k+1)^n}\,dx,$$

and the expression on the right-hand side is routine to evaluate:

$$\frac{N_n(\lambda)}{N_n(\mu)} = \frac{\Gamma(n-\frac{1}{k})}{\Gamma(n)\Gamma(1-\frac{1}{k})} = \prod_{m=1}^{n-1}\frac{km-1}{km}.$$

This product equals $-c(n,-k)$ divided by k^{2n-1}/n. $\square$

Remark 12.7.2. R. Stanley pointed out some interesting Schur function quotient results. See exercises 7.30 and 7.32 in [Sta99].

12.8 An integral from Gradshteyn and Ryzhik

It is now demonstrated how the previous results may be used to prove an integral evaluation found as entry 3.112 in [GR80]. The main tool is the (dual) Jacobi-Trudi identity which expresses a Schur function in terms of elementary symmetric functions. Namely, if λ is a partition such that its conjugate λ' (the unique partition whose Young diagram, see Section 12.6, is obtained from the one of λ by interchanging rows and columns) has length at most m then

$$s_\lambda = \left| e_{\lambda'_i - i + j} \right|_{1 \leqslant i,j \leqslant m}.$$

This identity may be found for instance in [Sta99, Corollary 7.16.2].

Theorem 12.8.1. *Let f_n and g_n be polynomials of the form*

$$\begin{aligned} g_n(x) &= b_0 x^{2n-2} + b_1 x^{2n-4} + \ldots + b_{n-1}, \\ f_n(x) &= a_0 x^n + a_1 x^{n-1} + \ldots + a_n, \end{aligned}$$

and assume that all roots of f_n lie in the upper half-plane. Then

$$\int_{-\infty}^{\infty} \frac{g_n(x)dx}{f_n(x)f_n(-x)} = \frac{\pi i}{a_0} \frac{M_n}{\Delta_n},$$

where

$$\Delta_n = \begin{vmatrix} a_1 & a_3 & a_5 & \ldots & 0 \\ a_0 & a_2 & a_4 & & 0 \\ 0 & a_1 & a_3 & & 0 \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & & a_n \end{vmatrix}, \qquad M_n = \begin{vmatrix} b_0 & b_1 & b_2 & \ldots & b_{n-1} \\ a_0 & a_2 & a_4 & & 0 \\ 0 & a_1 & a_3 & & 0 \\ \vdots & & & \ddots & \\ 0 & 0 & 0 & & a_n \end{vmatrix}.$$

Proof. Write $f_n(x) = a_0 \prod_{j=1}^n (x - iq_j)$. By assumption, Re $q_j > 0$. Further,

$$f_n(x)f_n(-x) = (-1)^n a_0^2 \prod_{j=1}^n (x^2 + q_j^2).$$

Let $\boldsymbol{q} = (q_1, q_2, \ldots, q_n)$. It follows from Theorem 12.5.4 that

$$\int_{-\infty}^{\infty} \frac{x^{2\beta} dx}{f_n(x) f_n(-x)} = \frac{(-1)^{n+\beta}\pi}{a_0^2} \frac{s_{\lambda(n-1)-2\beta\cdot\mathbf{1}^{n-1}}(\boldsymbol{q})}{s_{\lambda(n+1)-2\beta\cdot\mathbf{1}^{n}}(\boldsymbol{q})} = \frac{(-1)^{n}\pi}{a_0^2} \frac{s_{\lambda'}(\boldsymbol{q})}{s_{\lambda(n+1)}(\boldsymbol{q})}$$

where $\lambda = \lambda(n-1) + 2 \cdot \mathbf{1}^{\beta}$. The latter equality is obtained by writing the quotient of Schur functions as a quotient of alternants, multiplying the kth row of each matrix by $q_k^{2\beta}$, and reordering the columns of the determinant in the numerator. The right-hand side now is a quotient of Schur functions to which the Jacobi-Trudi identity may be applied. In the denominator, this gives

$$s_{\lambda(n+1)}(\boldsymbol{q}) = \left|e_{n+1-2k+j}(\boldsymbol{q})\right|_{1 \leqslant k,j \leqslant n} = \left|e_{2k-j}(\boldsymbol{q})\right|_{1 \leqslant k,j \leqslant n}.$$

Note that $e_m(\boldsymbol{q}) = 0$ whenever $m < 0$ or $m > n$. Further, $e_k(\boldsymbol{q}) = i^k a_k / a_0$. Hence, $s_{\lambda(n+1)}(\boldsymbol{q}) = i^{n(n+1)/2} \Delta_n / a_0^n$. The term $s_{\lambda'}(\boldsymbol{q})$ is dealt with analogously. The claim follows by expanding the determinant M_n with respect to the first row. $\square$

12.9 A sum related to Feynman diagrams

Particle scattering in quantum field theory is usually described in terms of Feynman diagrams. A Feynman diagram is a graphical representation of a particular term arising in the expansion of the relevant quantum-mechanical scattering amplitude as a power series in the coupling constants that parametrize the strengths of the interactions.

From the mathematical point of view, a Feynman diagram is a graph to which a certain function is associated. If the graph has circuits (*loops*, in the physics terminology) then this function is defined in terms of a number of integrals over the

4-dimensional momentum space $(k_0, \boldsymbol{k})$, where k_0 is the *energy* integration variable and $\boldsymbol{k}$ is a 3-dimensional *momentum* variable.

Feynman diagrams also appear in calculations of the thermodynamic properties of a system described by quantum fields. In this context, the integral over the energy component of a Feynman loop diagram is replaced by a summation over discrete energy values. These Matsubara sums were introduced in [Mat55]. A general method to compute these sums in terms of an associated integral was presented in [Esp10].

These techniques, applied to the expression (12.10) for the integral $G_n(\boldsymbol{q})$, give the value of the sum associated with the one-loop Feynman diagram consisting of n vertices and vanishing external momenta, $N_i = 0$, as depicted in Figure 12.2.

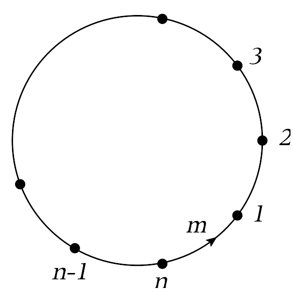

Figure 12.2: The one-loop Feynman diagram with n vertices and vanishing external momenta. m is the summation variable associated to each of the internal lines.

The Matsubara sum associated to the diagram in Figure 12.2 is

$$M_n(\boldsymbol{q}) := \sum_{m=-\infty}^{\infty} \prod_{k=1}^{n} \frac{1}{m^2 + q_k^2}, \tag{12.17}$$

where the variables q_k are related to the kinematic energies carried by the (virtual) particles in the Feynman diagram. This sum was denoted by S_G in [Esp10]; the notation has been changed here to avoid confusion.

Example 12.9.1. The first few Matsubara sums are

$$\begin{aligned}
M_1(q_1) &= \pi \frac{D_1}{q_1}, \\
M_2(q_1, q_2) &= \pi \frac{q_2 D_1 - q_1 D_2}{q_1 q_2 (q_2^2 - q_1^2)}, \\
M_3(q_1, q_2, q_3) &= \pi \frac{q_2 q_3 (q_2^2 - q_3^2) D_1 + q_3 q_1 (q_3^2 - q_1^2) D_2 + q_1 q_2 (q_1^2 - q_2^2) D_3}{q_1 q_2 q_3 (q_3^2 - q_2^2)(q_2^2 - q_1^2)(q_1^2 - q_3^2)},
\end{aligned}$$

with $D_j = \coth(\pi q_j)$.

Theorem 12.9.2. *The Matsubara sum $M_n(\boldsymbol{q})$ is given by*

$$M_n(\boldsymbol{q}) = \pi \sum_{k=1}^{n} \frac{\coth(\pi q_k)}{q_k} \prod_{\substack{j=1 \\ j \neq k}}^{n} \frac{1}{q_j^2 - q_k^2}.$$

Proof 1. This follows from the partial fraction expansion

$$\prod_{k=1}^{n} \frac{1}{m^2 + q_k^2} = \sum_{k=1}^{n} \frac{1}{q_k^2 + m^2} \prod_{j \neq k} \frac{1}{q_j^2 - q_k^2},$$

which is a special case of (12.11), switching the order of summation, and employing the classical

$$\frac{\pi \coth(\pi z)}{z} = \sum_{m=-\infty}^{\infty} \frac{1}{z^2 + m^2}.$$

□

Proof 2. The method developed in [Esp10] shows that

$$M_n(\boldsymbol{q}) = \pi \left[1 + \sum_{m=1}^{n} \mathrm{n_b}(q_m)(1 - R_m) \right] G_n(\boldsymbol{q}), \tag{12.18}$$

where $G_n(\boldsymbol{q})$ is the integral defined in (12.9),

$$\mathrm{n_b}(q) = \frac{1}{e^{2\pi q} - 1} = \frac{1}{2} \left(\coth \pi q - 1 \right),$$

and R_m is the reflection operator defined by

$$R_m f(q_1, \ldots, q_m, \ldots) = f(q_1, \ldots, -q_m, \ldots).$$

To use (12.18) combined with the evaluation (12.10) of $G_n(\boldsymbol{q})$ it is required to compute the action of each $1 - R_m$ on the summands of (12.10). Namely,

$$(1 - R_m)\frac{1}{q_k}\prod_{\substack{j=1\\j\neq k}}^{n}\frac{1}{q_j^2 - q_k^2} = \frac{2\delta_{km}}{q_k}\prod_{\substack{j=1\\j\neq k}}^{n}\frac{1}{q_j^2 - q_k^2},$$

where δ_{km} is the Kronecker delta. Therefore

$$\mathrm{n_b}(q_m)(1 - R_m)G_n(\boldsymbol{q}) = \frac{2\,\mathrm{n_b}(q_m)}{q_m}\prod_{\substack{j=1\\j\neq m}}^{n}\frac{1}{q_j^2 - q_m^2},$$

and the result follows from $2\,\mathrm{n_b}(q) = \coth(\pi q) - 1$. □

Finally, an expansion of $M_n(\boldsymbol{q})$ in terms of symmetric functions is given. Starting with the classical expansion

$$\frac{\pi \coth q_k}{q_k} = \frac{1}{q_k^2} - 2\sum_{m=1}^{\infty}(-1)^m q_k^{2m-2}\zeta(2m),$$

where $\zeta(s)$ denotes the Riemann zeta function, it follows that

$$M_n(\boldsymbol{q}) = \sum_{k=1}^{n}\frac{1}{q_k^2}\prod_{j\neq k}\frac{1}{q_j^2 - q_k^2} - 2\sum_{m=1}^{\infty}(-1)^m\zeta(2m)\sum_{k=1}^{n}q_k^{2(m-1)}\prod_{j\neq k}\frac{1}{q_j^2 - q_k^2}.$$

Using the identity (h_j being the complete homogeneous symmetric function)

$$h_{m-n}(x_1, \ldots, x_n) = (-1)^{n-1}\sum_{k=1}^{n}x_k^{m-1}\prod_{j\neq k}\frac{1}{x_j - x_k},$$

which follows from Lemma 12.5.3 (or see page 450, Exercise 7.4 of [Sta99]), this proves:

Corollary 12.9.3. *The Matsubara sum* $M_n(\boldsymbol{q})$*, defined in (12.17), is given by*

$$M_n(\boldsymbol{q}) = \frac{1}{e_n(\boldsymbol{q}^2)} + 2\sum_{m=0}^{\infty}(-1)^m \zeta(2m+2n) h_m(\boldsymbol{q}^2).$$

12.10 Conclusions

The evaluation of definite integrals has the charming quality of taking the reader for a tour of many parts of mathematics. An innocent-looking generalization of one of the oldest formulas in analysis has been shown to connect the work of the four authors in the title.

Chapter 13

A sinc that sank

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[BBS12] *A sinc that sank*
(with David Borwein, Jonathan M. Borwein)
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Abstract We resolve and further study a sinc integral evaluation, first posed in this MONTHLY in [1967, p. 1015], which was solved in [1968, p. 914] and withdrawn in [1970, p. 657]. After a short introduction to the problem and its history, we give a general evaluation which we make entirely explicit in the case of the product of three sinc functions. Finally, we exhibit some more general structure of the integrals in question.

13.1 Introduction and background

In [1967, #5529, p. 1015] D. Mitrinović asked in this MONTHLY for an evaluation of

$$I_n := \int_{-\infty}^{\infty} \prod_{j=1}^{n} \frac{\sin(k_j(x-a_j))}{x-a_j} \, \mathrm{d}x \tag{13.1}$$

for real numbers a_j, k_j with $1 \leqslant j \leqslant n$. We shall write $I_n\binom{a_1,\ldots,a_n}{k_1,\ldots,k_n}$ when we wish to emphasize the dependence on the parameters. Up to a constant factor, (13.1) is an integral over a product of sinc functions: $\operatorname{sinc} x := \frac{\sin x}{x}$.

The next year a solution [1968, #5529, p. 914] was published in the form of

$$I_n = \pi \prod_{j=2}^{n} \frac{\sin\left(k_j(a_1 - a_j)\right)}{a_1 - a_j} \tag{13.2}$$

under the assumption that $k_1 \geqslant k_2 \geqslant \ldots \geqslant k_n \geqslant 0$. This solution, as M. Klamkin pointed out in [1970, p. 657], can not be correct, since it is not symmetric in the parameters while I_n is. Indeed, in the case $k_1 = k_2 = k_3 = 1$ the evaluation (13.2) is not symmetric in the variables a_j and gives differing answers on permuting the a's. The proof given relies on formally correct Fourier analysis; but there are missing constraints on the k_j variables which have the effect that it is seldom right for more than two variables. Indeed, as shown then by D. Djoković and L. Glasser [Gla11] — who were both working in Waterloo at the time — the evaluation (13.2) holds true under the restriction $k_1 \geqslant k_2 + k_3 + \ldots + k_n$ when all of the k_j are positive. However, no simple general fix appeared possible — and indeed for $n > 2$ the issue is somewhat complex. The problem while recorded several times in later Monthly lists of unsolved problems appears (from a JSTOR hunt[1]) to have disappeared without trace in the later 1980's.

The precise issues regarding evaluation of sinc integrals are described in detail in [BB01] or [BBG04, Chapter 2] along with some remarkable consequences [BBB08, BB01, BBG04]. In the two-variable case, the 1968 solution is essentially correct; we do obtain

$$I_2 = \pi \frac{\sin\left((k_1 \wedge k_2)(a_1 - a_2)\right)}{a_1 - a_2} \tag{13.3}$$

[1]A search on JSTOR through all Monthly volumes, suggests that the solutions were never published and indeed for some years the original problem reappeared on lists of unsolved Monthly problems before apparently disappearing from view. Such a JSTOR search is not totally convincing since there is no complete indexing of problems and their status.

for $a_1 \neq a_2$ as will be made explicit below. Here $a \wedge b := \min\{a, b\}$. Some of the delicacy is a consequence of the fact that the classical sinc evaluation given next is only conditionally true [BB01]. We have

$$\int_{-\infty}^{\infty} \frac{\sin(kx)}{x}\,\mathrm{d}x = \pi\,\mathrm{sgn}(k), \tag{13.4}$$

where $\mathrm{sgn}(0) = 0, \mathrm{sgn}(k) = 1$ for $k > 0$ and $\mathrm{sgn}(k) = -1$ for $k < 0$.

In (13.4) the integral is absolutely divergent and is best interpreted as a Cauchy-Riemann limit. Thus the evaluation of (13.1) yields $I_1 = \pi\,\mathrm{sgn}(k_1)$ which has a discontinuity at $k_1 = 0$. For $n \geqslant 2$, however, I_n is an absolutely convergent integral which is (jointly) continuous as a function of all k_j and all a_j. This follows from Lebesgue's dominated convergence theorem since the absolute value of the integrand is less than $\prod_{j=1}^{n} |k_j|$ for all x and less than $2/x^2$ for all sufficiently large $|x|$.

It is worth observing that the oscillatory structure of the integrals, see Figure 13.1, means that their evaluation both numerically and symbolically calls for a significant amount of care.

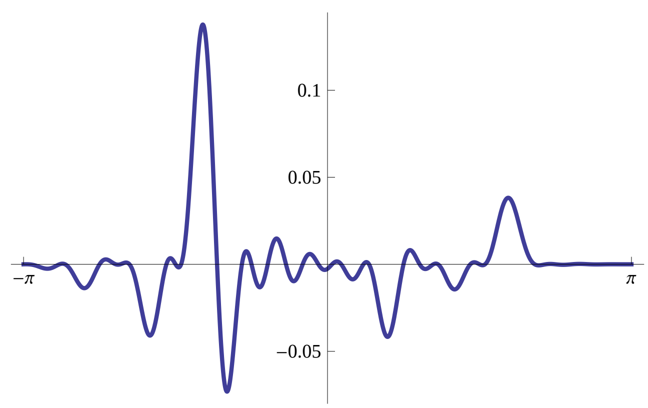

Figure 13.1: Integrand in (13.1) with $\mathbf{a} = (-3, -2, -1, 0, 1, 2)$, $\mathbf{k} = (1, 2, 3, 4, 5, 6)$

We wish to emphasize the continuing fascination with similar sinc integrals [GNJ87]. Indeed, the work in [BB01] was triggered by the exact problem described by K. Morrison in this MONTHLY [Mor95]. This led also to a lovely MONTHLY article on random series [Sch03], and there is further related work in [BG02].

A most satisfactory introduction to the many applications and properties of the sinc function is given in [GS90]. Additionally, T. Feeman's recent book on medical imaging [Fee10] chose to begin with the example given at the beginning of Section 13.4. The paper [MM08b] makes a careful and historically informed study of the geometric results implicit in the study of related multiple sinc integrals. This includes recording that G. Pólya in his 1912 doctoral thesis showed that if $k = (k_1, \ldots, k_n)$ has nonzero coefficients and

$$S_k(\theta) := \{x \in \mathbb{R}^n \ : \ |\langle k, x\rangle| \leqslant \theta/2, \, x \in C^n\}$$

denotes the slab inside the hypercube $C^n = \left[-\frac{1}{2}, \frac{1}{2}\right]^n$ cut off by the hyperplanes $\langle k, x\rangle = \pm\theta/2$, then

$$\mathrm{Vol}_n(S_k(\theta)) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\sin(\theta x)}{x} \prod_{j=1}^{n} \frac{\sin(k_j x)}{k_j x}\,\mathrm{d}x, \tag{13.5}$$

a relationship we return to in Section 13.4. More general polyhedra volumes determined by multidimensional sinc integrals are examined in [BBM02]. As a consequence of (13.5) and described for instance in [BB01], the integral (13.5) may also be interpreted as the probability that

$$\left|\sum_{j=1}^{n} k_j X_j\right| \leqslant \theta \tag{13.6}$$

where X_j are independent random variables uniformly distributed on $[-1, 1]$.

13.2 Evaluation of I_n

Without loss of generality, we assume that all k_j are strictly positive. In this section, we shall only consider the case when all the a_j are distinct. As illustrated in Sections 13.3.2 and 13.3.3, the special cases can be treated by taking limits. We begin with the classical and simple partial fraction expression

$$\prod_{j=1}^{n} \frac{1}{x-a_j} = \sum_{j=1}^{n} \frac{1}{x-a_j} \prod_{i\neq j} \frac{1}{a_j-a_i} \tag{13.7}$$

valid when the a_j are distinct. Applying (13.7) to the integral I_n we then have

$$\begin{aligned} I_n &= \sum_{j=1}^{n} \int_{-\infty}^{\infty} \frac{\sin(k_j(x-a_j))}{x-a_j} \prod_{i\neq j} \frac{\sin(k_i(x-a_i))}{a_j-a_i}\,\mathrm{d}x \\ &= \sum_{j=1}^{n} \int_{-\infty}^{\infty} \frac{\sin(k_j x)}{x} \prod_{i\neq j} \frac{\sin(k_i(x+(a_j-a_i)))}{a_j-a_i}\,\mathrm{d}x. \end{aligned} \tag{13.8}$$

We pause and illustrate the general approach in the case of $n=2$ variables.

Example 13.2.1 (Two variables)**.** We apply (13.8) to write

$$\begin{aligned} I_2 &= \int_{-\infty}^{\infty} \frac{\sin(k_1 x)}{x}\,\frac{\sin\left(k_2(x+a_1-a_2)\right)}{a_2-a_1}\,\mathrm{d}x \\ &\quad + \int_{-\infty}^{\infty} \frac{\sin(k_2 x)}{x}\,\frac{\sin\left(k_1(x+a_2-a_1)\right)}{a_1-a_2}\,\mathrm{d}x \\ &= \frac{\sin\left(k_2(a_1-a_2)\right)}{a_1-a_2} \int_{-\infty}^{\infty} \frac{\sin(k_1 x)}{x} \cos(k_2 x)\,\mathrm{d}x \\ &\quad + \frac{\sin\left(k_1(a_2-a_1)\right)}{a_2-a_1} \int_{-\infty}^{\infty} \frac{\sin(k_2 x)}{x} \cos(k_1 x)\,\mathrm{d}x \end{aligned}$$

where for the second equation we have used the addition formula for the sine and noticed that the sine-only integrands (being odd) integrate to zero. Finally, we either appeal to [BB01, Theorem 3] or express

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{\sin(k_1 x)}{x} \cos(k_2 x)\,\mathrm{d}x &= \frac{1}{2} \int_{-\infty}^{\infty} \frac{\sin\left((k_1+k_2)x\right)}{x}\,\mathrm{d}x \\ &\quad + \frac{1}{2} \int_{-\infty}^{\infty} \frac{\sin\left((k_1-k_2)x\right)}{x}\,\mathrm{d}x, \end{aligned}$$

and appeal twice to (13.4) to obtain the final elegant cancellation

$$I_2 = \pi \, \frac{\sin\left((k_1 \wedge k_2)(a_1 - a_2)\right)}{a_1 - a_2} \tag{13.9}$$

valid for $a_1 \neq a_2$. We observe that the result remains true for $a_1 = a_2$, in which case the right-hand side of (13.9) attains the limiting value $\pi(k_1 \wedge k_2)$. $\Diamond$

Let us observe that after the first step in Example 13.2.1 — independent of the exact final formula — the integrals to be obtained have lost their dependence on the a_j. This is what we exploit more generally. Proceeding as in Example 13.2.1 and applying the addition formula to (13.8) we write,

$$I_n = \sum_{j=1}^{n} \sum_{A,B} C_{j,A,B} \; \alpha_{j,A,B} \tag{13.10}$$

where the sum is over all sets A and B partitioning $\{1, 2 \ldots, j-1, j+1, \ldots n\}$, and

$$C_{j,A,B} := \prod_{i \in A} \frac{\cos(k_i(a_j - a_i))}{a_j - a_i} \prod_{i \in B} \frac{\sin(k_i(a_j - a_i))}{a_j - a_i} \tag{13.11}$$

while

$$\alpha_{j,A,B} := \int_{-\infty}^{\infty} \prod_{i \in A \cup \{j\}} \sin(k_i x) \prod_{i \in B} \cos(k_i x) \, \frac{\mathrm{d}x}{x}. \tag{13.12}$$

Notice that we may assume the cardinality $|A|$ of A to be even since the integral in (13.12) vanishes if $|A|$ is odd.

To further treat (13.10), we write the products of sines and cosines in terms of sums of single trigonometric functions. The general formulae are made explicit next.

Proposition 13.2.2 (Cosine product)**.**

$$\prod_{j=1}^{r} \cos(x_j) = 2^{-r} \sum_{\varepsilon\in\{-1,1\}^r} \cos\left(\sum_{j=1}^{r} \varepsilon_j x_j\right). \tag{13.13}$$

Proof. The formula follows from the trigonometric identity $2\cos(a)\cos(b) = \cos(a+b) + \cos(a-b)$ applied inductively. □

Observe that by taking derivatives with respect to some of the x_j in (13.13), we obtain similar formulae for general products of sines and cosines.

Corollary 13.2.3 (Sine and cosine product)**.**

$$\prod_{j=1}^{s} \sin(x_j) \prod_{j=s+1}^{r} \cos(x_j) = 2^{-r} \sum_{\varepsilon\in\{-1,1\}^r} \left(\prod_{j=1}^{s} \varepsilon_i\right) \cos\left(\sum_{j=1}^{r} \varepsilon_j x_j - \frac{s\pi}{2}\right). \tag{13.14}$$

Here, we used $\frac{\mathrm{d}}{\mathrm{d}x}\cos(x) = \cos(x-\pi/2)$ to write the evaluation rather compactly. Note that when $s = 2k+1$ is odd then $\cos(x - s\pi/2) = (-1)^k \sin(x)$. Applying (13.14) to the definition (13.12), it thus follows that, for even $|A|$,

$$\begin{aligned} \alpha_{j,A,B} &= (-1)^{|A|/2} \int_{-\infty}^{\infty} \frac{1}{2^n} \sum_{\varepsilon\in\{-1,1\}^n} \left(\prod_{i\in A\cup\{j\}} \varepsilon_i\right) \sin\left(\sum_{i=1}^{n} \varepsilon_i k_i x\right) \frac{\mathrm{d}x}{x} \\ &= \pi\,(-1)^{|A|/2} \frac{1}{2^n} \sum_{\varepsilon\in\{-1,1\}^n} \left(\prod_{i\in A\cup\{j\}} \varepsilon_i\right) \operatorname{sgn}\left(\sum_{i=1}^{n} \varepsilon_i k_i\right). \end{aligned} \tag{13.15}$$

Then, on combining (13.15) with (13.10), we obtain the following general evaluation.

Theorem 13.2.4 (General evaluation)**.** *We have*

$$I_n = \sum_{j=1}^{n} \sum_{A,B} \alpha_{j,A,B}\, C_{j,A,B} \tag{13.16}$$

where the inner summation is over disjoint sets A, B such that $|A|$ is even and $A \cup B = \{1, 2, \ldots, j-1, j+1, \ldots, n\}$. The trigonometric products

$$C_{j,A,B} = \prod_{i \in A} \frac{\cos(k_i(a_j - a_i))}{a_j - a_i} \prod_{i \in B} \frac{\sin(k_i(a_j - a_i))}{a_j - a_i}$$

are as in (13.11) *and* $\alpha_{j,A,B}$ *is given by* (13.15).

Note that in dimension $n \geqslant 2$, there are $n2^{n-2}$ elements $C_{j,A,B}$ which may or may not be distinct.

Remark 13.2.5. Note that, just like for the defining integral for I_n, it is apparent that the terms $C_{j,A,B}$ and hence the evaluation of I_n given in (13.16) only depend on the parameters a_j up to a common shift. In particular, setting $b_j = a_j - a_n$ for $j = 1, \ldots, n-1$ the evaluation in (13.16) can be written as a symmetric function in the $n-1$ variables b_j. $\Diamond$

As an immediate consequence of Theorem 13.2.4 we have:

Corollary 13.2.6 (Simplest case)**.** *Assume, without loss, that* $k_1, k_2, \ldots, k_n > 0$. *Suppose that there is an index* ℓ *such that*

$$k_\ell > \frac{1}{2} \sum k_i.$$

In that case, the original solution to the Monthly *problem is valid; that is,*

$$I_n = \int_{-\infty}^{\infty} \prod_{i=1}^{n} \frac{\sin(k_i(x - a_i))}{x - a_i} \mathrm{d}x = \pi \prod_{i \neq \ell} \frac{\sin(k_i(a_\ell - a_i))}{a_\ell - a_i}.$$

This result was independently obtained by Djoković and Glasser [Gla11].

Proof. In this case,

$$\operatorname{sgn}\left(\sum_{i=1}^{n} \varepsilon_i k_i\right) = \varepsilon_\ell$$

for all values of the ε_i. The claim now follows from Theorem 13.2.4. More precisely, if there is some index $k \neq \ell$ such that $k \in A$ or $j = k$, then $\alpha_{j,A,B} = 0$. This is because the term in (13.15) contributed by $\varepsilon \in \{-1,1\}^n$ has opposite sign than the term contributed by ε', where ε' is obtained from ε by flipping the sign of ε_k. It remains to observe that $\alpha_{\ell,\emptyset,B} = \pi$ according to (13.15). This is the only surviving term. $\square$

13.2.1 Alternative evaluation of I_n

In 1970 Djoković sent in a solution to the MONTHLY after the original solution was withdrawn [Gla11]. He used the following identity involving the principal value (PV) of the integral

$$\text{(PV)} \int_{-\infty}^{\infty} \frac{e^{itx}}{x-a_j} \mathrm{d}x = \lim_{\delta\to 0+} \left\{ \int_{-\infty}^{a_j-\delta} + \int_{a_j+\delta}^{\infty} \right\} \frac{e^{itx}}{x-a_j} \mathrm{d}x = \pi i \operatorname{sgn}(t) e^{ita_j}$$

where t is real. Note that setting $a_j = 0$ and taking the imaginary part gives (13.4). He then showed, using the same partial fraction expansion as above, that

$$\begin{aligned} I_n = \frac{\pi i}{(2i)^n} \sum_{j=1}^{n} \Bigg\{ A_j \sum_{\varepsilon \in \{-1,1\}^n} \left(\prod_{r=1}^{n} \varepsilon_r \right) \operatorname{sgn} \left(\sum_{r=1}^{n} \varepsilon_r k_r \right) \\ \cdot \exp \left(i \sum_{r=1}^{n} \varepsilon_r k_r (a_j - a_r) \right) \Bigg\} \end{aligned} \tag{13.17}$$

where $a_1, a_2, \ldots, a_n$ are distinct and

$$A_j := \frac{1}{\prod_{r\neq j}(a_j - a_r)}. \tag{13.18}$$

The formula (13.17) is quite elegant and also allows one to derive Corollary 13.2.6, which was independently found by Glasser [Gla11]. For instance, it suffices to appeal to the case $r = s$ of (13.14). However, as we will demonstrate in the remainder, the evaluation given in Theorem 13.2.4 has the advantage of making significant additional structure of the integrals I_n more apparent. Before doing so in Section 13.5 we next consider the case I_3 in detail.

13.3 The case $n = 3$

We can completely dispose of the three-dimensional integral I_3 by considering the three cases: a_1, a_2, a_3 distinct; a_1 distinct from $a_2 = a_3$; and $a_1 = a_2 = a_3$.

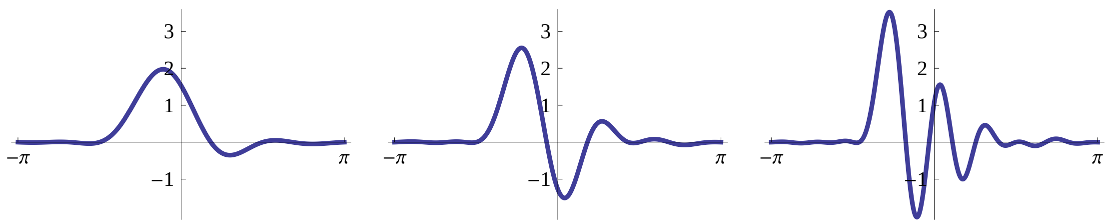

Figure 13.2: Integrands in (13.1) with parameters $\mathbf{a} = (-1, 0, 1)$ and $\mathbf{k} = (k_1, 2, 1)$ where $k_1 = 2, 4, 7$

13.3.1 The case $n = 3$ when a_1, a_2, a_3 are distinct

As demonstrated in this section, the evaluation of I_3 will depend on which inequalities are satisfied by the parameters k_1, k_2, k_3. For $n = 3$, Theorem 13.2.4 yields:

$$I_3\binom{a_1, a_2, a_3}{k_1, k_2, k_3} = \frac{1}{8}\sum_{j=1}^{3}\sum_{\varepsilon\in\{-1,1\}^3}\left[\varepsilon_j \operatorname{sgn}(\varepsilon_1 k_1 + \varepsilon_2 k_2 + \varepsilon_3 k_3)\prod_{i\neq j}\frac{\sin(k_i(a_j - a_i))}{a_j - a_i}\right.$$
$$\left. - \varepsilon_1\varepsilon_2\varepsilon_3 \operatorname{sgn}(\varepsilon_1 k_1 + \varepsilon_2 k_2 + \varepsilon_3 k_3)\prod_{i\neq j}\frac{\cos(k_i(a_j - a_i))}{a_j - a_i}\right]. \quad (13.19)$$

Remark 13.3.1 (Recovering Djoković's evaluation)**.** Upon using the trigonometric identity $\sin(x)\sin(y) - \cos(x)\cos(y) = -\cos(x+y)$ to combine the two products, the right-hand side of equation (13.19) can be reexpressed in the symmetric form

$$-\frac{1}{8}\sum_{\varepsilon\in\{-1,1\}^3} \varepsilon_1\varepsilon_2\varepsilon_3 \operatorname{sgn}(\varepsilon_1 k_1 + \varepsilon_2 k_2 + \varepsilon_3 k_3) \sum_{j=1}^{3} \frac{\cos(\sum_{i\neq j} \varepsilon_i k_i (a_j - a_i))}{\prod_{i\neq j}(a_j - a_i)}.$$

This is precisely Djoković's evaluation (13.17). ♢

In fact, distinguishing between two cases, illustrated in Figure 13.3, the evaluation (13.19) of I_3 can be made entirely explicit:

Corollary 13.3.2 (a_1, a_2, a_3 distinct)**.** *Assume that* $k_1, k_2, k_3 > 0$. *Then*

1. *If* $\frac{1}{2}\sum k_i \leqslant k_\ell$, *as can happen for at most one index* ℓ, *then*

$$I_3\binom{a_1, a_2, a_3}{k_1, k_2, k_3} = \pi \prod_{i\neq \ell} \frac{\sin(k_i(a_\ell - a_i))}{a_\ell - a_i}. \tag{13.20}$$

2. *Otherwise, that is if* $\max k_i < \frac{1}{2}\sum k_i$, *then*

$$I_3\binom{a_1, a_2, a_3}{k_1, k_2, k_3} = \frac{\pi}{2}\sum_{j=1}^{3}\left[\prod_{i\neq j}\frac{\sin(k_i(a_j - a_i))}{a_j - a_i} + \prod_{i\neq j}\frac{\cos(k_i(a_j - a_i))}{a_j - a_i}\right]. \tag{13.21}$$

Proof. The first case is a special case of Corollary 13.2.6. Alternatively, assuming without loss that the inequality for k_ℓ is strict, it follows directly from (13.19) (because $\operatorname{sgn}(\varepsilon_1 k_1 + \varepsilon_2 k_2 + \varepsilon_3 k_3) = \varepsilon_\ell$, all but one sum over $\varepsilon \in \{-1, 1\}^3$ cancel to zero).

In the second case, $k_1 < k_2 + k_3$, $k_2 < k_3 + k_1$, $k_3 < k_1 + k_2$. Therefore

$$\frac{1}{8}\sum_{\varepsilon\in\{-1,1\}^3} \varepsilon_j \operatorname{sgn}(\varepsilon_1 k_1 + \varepsilon_2 k_2 + \varepsilon_3 k_3) = \frac{1}{2} \quad \text{for all } j,$$

$$-\frac{1}{8}\sum_{\varepsilon\in\{-1,1\}^3} \varepsilon_1\varepsilon_2\varepsilon_3 \operatorname{sgn}(\varepsilon_1 k_1 + \varepsilon_2 k_2 + \varepsilon_3 k_3) = \frac{1}{2}.$$

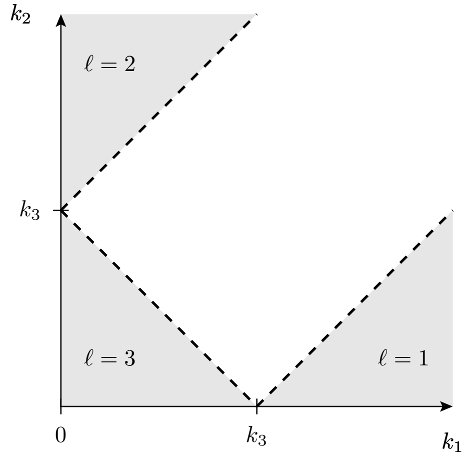

Figure 13.3: The constraints on the parameters k_j in Corollary 13.3.2 — if k_1, k_2 take values in the shaded regions then (13.20) holds with the indicated choice of ℓ

The claim then follows from (13.19). □

Remark 13.3.3 (Hidden trigonometric identities)**.** Observe that because of the continuity of I_3 as a function of k_1, k_2, and k_3, we must have the nonobvious identity

$$\prod_{i\neq 1}\left[\frac{\sin(k_i(a_1-a_i))}{a_1-a_i}\right]=\frac{1}{2}\sum_{j=1}^{3}\left[\prod_{i\neq j}\frac{\sin(k_i(a_j-a_i))}{a_j-a_i}+\prod_{i\neq j}\frac{\cos(k_i(a_j-a_i))}{a_j-a_i}\right] \tag{13.22}$$

when $k_1 = k_2 + k_3$. We record that *Mathematica 7* is able to verify (13.22); however, it struggles with the analogous identities arising for $n \geqslant 4$. ♢

13.3.2 The case $n = 3$ when $a_1 \neq a_2 = a_3$

As a limiting case of Corollary 13.3.2 we obtain the following.

Corollary 13.3.4 ($a_1 \neq a_2 = a_3$)**.** *Assume that* $k_1, k_2, k_3 > 0$ *and* $a_1 \neq a_2$*. Set* $a := a_2 - a_1$*.*

1. *If* $k_1 \geqslant \frac{1}{2}\sum k_i$*, then*

$$I_3\begin{pmatrix} a_1, a_2, a_2 \\ k_1, k_2, k_3 \end{pmatrix} = \pi \frac{\sin(k_2 a)}{a}\frac{\sin(k_3 a)}{a}. \tag{13.23}$$

2. *If* $\max(k_2, k_3) \geqslant \frac{1}{2}\sum k_i$*, then*

$$I_3\begin{pmatrix} a_1, a_2, a_2 \\ k_1, k_2, k_3 \end{pmatrix} = \pi \min(k_2, k_3)\frac{\sin(k_1 a)}{a}. \tag{13.24}$$

3. *Otherwise, that is if* $\max k_i < \frac{1}{2}\sum k_i$*, then*

$$I_3\begin{pmatrix} a_1, a_2, a_2 \\ k_1, k_2, k_3 \end{pmatrix} = \frac{\pi}{2}\frac{\cos((k_2-k_3)a)-\cos(k_1 a)}{a^2} + \frac{\pi}{2}\frac{(k_2+k_3-k_1)\sin(k_1 a)}{a}. \tag{13.25}$$

Proof. The first two cases are immediate consequences of (13.20) upon taking the limit $a_3 \to a_2$.

Likewise, the third case follows from (13.21) with just a little bit of care. The contribution of the sine products from (13.21) is

$$\frac{\pi}{2}\frac{\sin(k_2 a)\sin(k_3 a)}{a^2} + \frac{\pi}{2}\frac{(k_2+k_3)\sin(k_1 a)}{a}.$$

On the other hand, writing $a_3 = a_2 + \varepsilon$ with the intent of letting $\varepsilon \to 0$, the cosine products contribute

$$\frac{\pi}{2}\left[\frac{\cos(k_2 a)\cos(k_3 a)}{a^2} - \frac{\cos(k_1 a)\cos(k_3 \varepsilon)}{a\varepsilon} + \frac{\cos(k_1(a+\varepsilon))\cos(k_2\varepsilon)}{(a+\varepsilon)\varepsilon}\right].$$

The claim therefore follows once we show

$$\frac{\cos(k_1 a)\cos(k_3\varepsilon)}{a\varepsilon} - \frac{\cos(k_1(a+\varepsilon))\cos(k_2\varepsilon)}{(a+\varepsilon)\varepsilon} \to \frac{\cos(k_1 a)}{a^2} + \frac{k_1\sin(k_1 a)}{a}.$$

This is easily verified by expanding the left-hand side in a Taylor series with respect to ε. In fact, all the steps in this proof can be done automatically using, for instance, *Mathematica 7*. □

Observe that, since I_n is invariant under changing the order of its arguments, Corollary 13.3.4 covers all cases where exactly two of the parameters a_j agree.

Remark 13.3.5 (Alternative approach)**.** We remark that Corollary 13.3.4 can alternatively be proved in analogy with the proof given for Theorem 13.2.4 — that is by starting with a partial fraction decomposition and evaluating the occurring basic integrals. Besides integrals covered by equation (13.15), this includes formulae such as

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{\sin(k_2 x)}{x} \frac{\sin(k_3 x)}{x} \cos(k_1 x) \mathrm{d}x \\ = \frac{\pi}{8} \sum_{\varepsilon \in \{-1,1\}^3} \varepsilon_2 \varepsilon_3 (\varepsilon_1 k_1 + \varepsilon_2 k_2 + \varepsilon_3 k_3) \operatorname{sgn}(\varepsilon_1 k_1 + \varepsilon_2 k_2 + \varepsilon_3 k_3).\end{aligned} \tag{13.26}$$

This evaluation follows from [BB01, Theorem 3(ii)]. In fact, (13.26) is an immediate consequence of equation (13.15) with $n = 3$ and $A = \emptyset$ after integrating with respect to one of the parameters k_i where $i \in B$. Clearly, this strategy evaluates a large class of integrals, similar to (13.26), over the real line with integrands products of sines and cosines as well as powers of the integration variable (see also [BB01]). ♢

13.3.3 The case $n = 3$ when $a_1 = a_2 = a_3$

In this case,

$$\begin{aligned} I_3 &= \int_{-\infty}^{\infty} \frac{\sin(k_1(x-a_1))}{x-a_1} \frac{\sin(k_2(x-a_1))}{x-a_1} \frac{\sin(k_3(x-a_1))}{x-a_1} \mathrm{d}x \\ &= \int_{-\infty}^{\infty} \frac{\sin(k_1 x)}{x} \frac{\sin(k_2 x)}{x} \frac{\sin(k_3 x)}{x} \mathrm{d}x. \end{aligned} \tag{13.27}$$

Corollary 13.3.6 ($a_1 = a_2 = a_3$). *Assume, without loss, that $k_1 \geqslant k_2 \geqslant k_3 > 0$. Then*

1. *If $k_1 \geqslant k_2 + k_3$, then*
$$I_3 \binom{a_1, a_1, a_1}{k_1, k_2, k_3} = \pi\, k_2 k_3.$$

2. *If $k_1 \leqslant k_2 + k_3$, then*

$$I_3 \binom{a_1, a_1, a_1}{k_1, k_2, k_3} = \pi \left(k_2 k_3 - \frac{(k_2 + k_3 - k_1)^2}{4} \right).$$

Proof. The first part follows from Theorem 2 and the second from Corollary 1 in [BB01].

Alternatively, Corollary 13.3.6 may be derived from Corollary 13.3.4 on letting a tend to zero. Again, this can be automatically done in a computer algebra system such as *Mathematica 7* or *Maple 14*. □

13.4 Especially special cases of sinc integrals

The same phenomenon as in equation (13.5) and in Corollary 13.3.6 leads to one of the most striking examples in [BB01]. Consider the following example of a re-normalized I_n integral, in which we set

$$J_n := \int_{-\infty}^{\infty} \operatorname{sinc} x \cdot \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{2n+1}\right) \mathrm{d}x.$$

Then — as *Maple* and *Mathematica* are able to confirm — we have the following evaluations:

$$\begin{aligned}
J_0 &= \int_{-\infty}^{\infty} \operatorname{sinc} x \,\mathrm{d}x = \pi,\\
J_1 &= \int_{-\infty}^{\infty} \operatorname{sinc} x \cdot \operatorname{sinc}\left(\frac{x}{3}\right)\,\mathrm{d}x = \pi,\\
&\ \vdots\\
J_6 &= \int_{-\infty}^{\infty} \operatorname{sinc} x \cdot \operatorname{sinc}\left(\frac{x}{3}\right)\cdots \operatorname{sinc}\left(\frac{x}{13}\right)\,\mathrm{d}x = \pi.
\end{aligned}$$

As explained in detail in [BB01] or [BBG04, Chapter 2], the seemingly obvious pattern — a consequence of Corollary 13.2.6 — is then confounded by

$$\begin{aligned}
J_7 &= \int_{-\infty}^{\infty} \operatorname{sinc} x \cdot \operatorname{sinc}\left(\frac{x}{3}\right)\cdots \operatorname{sinc}\left(\frac{x}{15}\right)\,\mathrm{d}x\\
&= \frac{467807924713440738696537864469}{467807924720320453655260875000}\pi < \pi,
\end{aligned}$$

where the fraction is approximately $0.99999999998529\ldots$ which, depending on the precision of calculation, numerically might not even be distinguished from 1.

This is a consequence of the following general evaluation given in [BB01].

Theorem 13.4.1 (First bite)**.** *Denote $K_m = k_0 + k_1 + \ldots + k_m$. If $2k_j \geqslant k_n > 0$ for $j = 0, 1, \ldots, n-1$ and $K_n > 2k_0 \geqslant K_{n-1}$, then*

$$\int_{-\infty}^{\infty} \prod_{j=0}^{n} \frac{\sin(k_j x)}{x}\,\mathrm{d}x = \pi k_1 k_2 \cdots k_n - \frac{\pi}{2^{n-1} n!}(K_n - 2k_0)^n. \tag{13.28}$$

Note that Theorem 13.4.1 is a "first-bite" extension of Corollary 13.2.6; assuming only that $k_j > 0$ for $j = 0, 1, \ldots, n$ then if $2k_0 > K_n$ the integral evaluates to $\pi k_1 k_2 \cdots k_n$.

Theorem 13.4.1 makes clear that the pattern $J_n = \pi$ for $n = 0, 1, \ldots, 6$ breaks for J_7 because

$$\frac{1}{3} + \frac{1}{5} + \ldots + \frac{1}{15} > 1$$

whereas all earlier partial sums are less than 1. Geometrically, the situation is as follows. In light of (13.5), the integral J_n may be interpreted as the volume of the part of a hypercube lying between two planes. For $n = 7$ these planes intersect with the hypercube for the first time.

Example 13.4.2 (A probabilistic interpretation)**.** Let us illustrate Theorem 13.4.1 using the probabilistic point of view mentioned in (13.6) at the end of the introduction. As such the integral

$$\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\sin(k_0 x)}{x}\frac{\sin(k_1 x)}{k_1 x}\frac{\sin(k_2 x)}{k_2 x}\,\mathrm{d}x$$

is the probability that $|k_1 X_1 + k_2 X_2| \leqslant k_0$ where X_1, X_2 are independent random variables distributed uniformly on $[-1, 1]$.

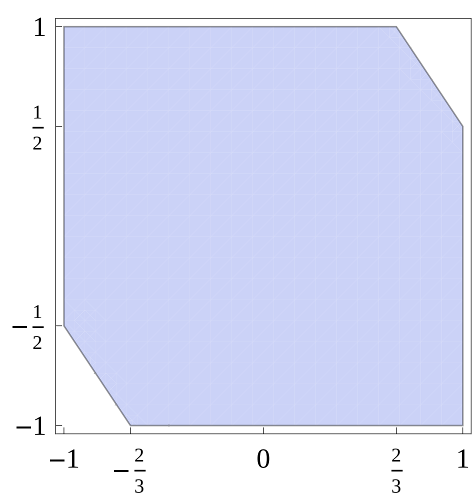

Figure 13.4: The event $|3X_1 + 2X_2| \leqslant 4$

In the case $k_0 = 4$, $k_1 = 3$, $k_2 = 2$, for example, this event is represented as the shaded area in Figure 13.4. Since each of the removed triangular corners has sides of length 1/2 and 1/3, this region has area 23/6. Because the total area is 4, the probability of the event in question is 23/24. Thus,

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\sin(4x)}{x}\frac{\sin(3x)}{3x}\frac{\sin(2x)}{2x}\,\mathrm{d}x=\frac{23}{24}=\frac{1}{3\cdot 2}\left(3\cdot 2-\frac{(3+2-4)^2}{2\cdot 2}\right)$$

in agreement with Theorem 13.4.1. ♢

Let us return to the example of the integrals J_n. Even past $n=7$, we do have a surprising equality [BBB08] of these integrals and corresponding Riemann sums. This alternative evaluation of the integrals J_n is

$$\int_{-\infty}^{\infty}\prod_{j=0}^{n}\operatorname{sinc}\left(\frac{x}{2j+1}\right)\mathrm{d}x=\sum_{m=-\infty}^{\infty}\prod_{j=0}^{n}\operatorname{sinc}\left(\frac{m}{2j+1}\right) \tag{13.29}$$

which is valid for $n=1,2,\ldots,7,8,\ldots,40248$. The "first-bite" phenomenon is seen here again but at larger n. For $n>40248$ this equality fails as well; the sum being strictly bigger than the integral. As in the case of (13.28), there is nothing special about the choice of parameters $k_j=\frac{1}{2j+1}$ in the sinc functions. Indeed, the following general result is proved in [BBB08].

Theorem 13.4.3. *Suppose that $k_1,k_2,\ldots,k_n>0$. If $k_1+k_2+\ldots+k_n<2\pi$, then*

$$\int_{-\infty}^{\infty}\prod_{j=1}^{n}\operatorname{sinc}(k_jx)\,\mathrm{d}x=\sum_{m=-\infty}^{\infty}\prod_{j=1}^{n}\operatorname{sinc}(k_jm). \tag{13.30}$$

Note that the condition $k_1+k_2+\ldots+k_n<2\pi$ may always be satisfied through a common rescaling $k_j\to\tau k_j$ of the parameters k_j at the expense of writing the sinc integral as a sinc sum with differently scaled parameters.

As a consequence of Theorem 13.4.3, we see that (13.29) holds for n provided that

$$\sum_{j=0}^{n}\frac{1}{2j+1}<2\pi$$

which is true precisely for the range of n specified above.

Remark 13.4.4. With this insight, it is not hard to contrive more persistent examples. An entertaining example given in [BBB08] is taking the reciprocals of primes. Using the Prime Number Theorem, one estimates that the sinc integrals equal the sinc sums until the number of products is about 10^{176}. That of course makes it rather unlikely to find, by mere testing, an example where the two are unequal. Even worse for the naive tester is the fact that the discrepancy between integral and sum is always less than $10^{-10^{86}}$ (and even smaller if the Riemann hypothesis is true). $\diamondsuit$

A related integral, which because of its varied applications has appeared repeatedly in the literature, see e.g. [MR65] and the references therein, is

$$\frac{2}{\pi}\int_0^\infty \left(\frac{\sin x}{x}\right)^n \cos(bx)\,\mathrm{d}x \tag{13.31}$$

which, for $0 \leqslant b < n$, has the closed form

$$\frac{1}{2^{n-1}(n-1)!}\sum_{0\leqslant k<(n+b)/2}(-1)^k\binom{n}{k}(n+b-2k)^{n-1}.$$

To give an idea of the range of applications, we only note that the authors of [MR65] considered the integral (13.31) because it is proportional to "the intermodulation distortion generated by taking the nth power of a narrow-band, high-frequency white noise"; on the other hand, the recent [Ali08] uses (13.31) with $b = 0$ to obtain an improved lower bound for the Erdős-Moser problem.

If $b \geqslant n$, then the integral (13.31) vanishes. The case $b = 0$ in (13.31) is the interesting special case of I_n with $k_1 = \ldots = k_n = 1$ and $a_1, \ldots, a_n = 0$. Its evaluation appears as an exercise in [WW27, p. 123]; in [BB01] it is demonstrated how it may be derived using the present methods.

13.5 The case $n \geqslant 4$

Returning to Theorem 13.2.4, we now show — somewhat briefly — that in certain general cases the evaluation of the integral I_n may in essence be reduced to the evaluation of the integral I_m for some $m < n$. In particular, we will see that Corollary 13.2.6 is the most basic such case — corresponding to $m = 1$.

In order to exhibit this general structure of the integrals I_n, we introduce the notation

$$I_{n,j} := \sum_{A,B} \alpha_{j,A,B}\, C_{j,A,B} \tag{13.32}$$

so that, by (13.16), $I_n = \sum_{j=1}^{n} I_{n,j}$.

Theorem 13.5.1 (Substructure)**.** *Assume that $k_1 \geqslant k_2 \geqslant \ldots \geqslant k_n > 0$, and that $a_1, a_2, \ldots, a_n$ are distinct. Suppose that there is some m such that for all $\varepsilon \in \{-1, 1\}^n$ we have*

$$\operatorname{sgn}(\varepsilon_1 k_1 + \ldots + \varepsilon_m k_m + \ldots + \varepsilon_n k_n) = \operatorname{sgn}(\varepsilon_1 k_1 + \ldots + \varepsilon_m k_m). \tag{13.33}$$

Then

$$I_n = \sum_{j=1}^{m} I_{m,j} \prod_{i>m} \frac{\sin(k_i(a_j - a_i))}{a_j - a_i}. \tag{13.34}$$

Proof. Note that in light of (13.15) and (13.33) we have $\alpha_{j,A,B} = 0$ unless $\{m + 1, \ldots, n\} \subset B$. To see this, assume that there is some index $k > m$ such that $k \in A$ or $k = j$. Then the term in (13.15) contributed by $\varepsilon \in \{-1, 1\}^n$ has opposite sign as the term contributed by ε', where ε' is obtained from ε by flipping the sign of ε_k. The claim now follows from Theorem 13.2.4. $\square$

Remark 13.5.2. The condition (13.33) may equivalently be stated as

$$\min |\varepsilon_1 k_1 + \ldots + \varepsilon_m k_m| > k_{m+1} + \ldots + k_n \tag{13.35}$$

where the minimum is taken over $\varepsilon \in \{-1, 1\}^m$. We idly remark that, for large m, computing this minimum is a hard problem. In fact, in the special case of integral k_j, just deciding whether the minimum is zero (which is equivalent to the *partition problem* of deciding whether the parameters k_j can be partitioned into two sets with the same sum) is well-known to be NP-complete [GJ79, Section 3.1.5]. ♢

Observe that the case $m = 1$ of Theorem 13.5.1, together with the basic evaluation (13.4), immediately implies Corollary 13.2.6. This is because the condition (13.33) holds for $m = 1$ precisely if $k_1 > k_2 + \ldots + k_n$.

If (13.33) holds for $m = 2$, then it actually holds for $m = 1$ provided that the assumed inequality $k_1 \geqslant k_2$ is strict. Therefore the next interesting case is $m = 3$. The final evaluation makes this case explicit. It follows from Corollary 13.3.2.

Corollary 13.5.3 (A second n-dimensional case)**.** *Let $n \geqslant 3$. Assume that $k_1 \geqslant k_2 \geqslant \ldots \geqslant k_n > 0$, and that $a_1, a_2, \ldots, a_n$ are distinct. If*

$$k_1 \leqslant k_2 + \ldots + k_n \quad \textit{and} \quad k_2 + k_3 - k_1 \geqslant k_4 + \ldots + k_n,$$

then

$$I_n = \frac{\pi}{2} \sum_{j=1}^{3} \prod_{i \geqslant 4} \frac{\sin(k_i(a_j - a_i))}{a_j - a_i} \left[\prod_{i \leqslant 3, i \neq j} \frac{\sin(k_i(a_j - a_i))}{a_j - a_i} + \prod_{i \leqslant 3, i \neq j} \frac{\cos(k_i(a_j - a_i))}{a_j - a_i} \right].$$

The cases $m \geqslant 4$ quickly become much more involved. In particular, the condition (13.33) becomes a set of inequalities. To close, we illustrate with the first case not covered by Corollaries 13.2.6 and 13.5.3:

Example 13.5.4. As usual, assume that $k_1 \geqslant k_2 \geqslant k_3 \geqslant k_4 > 0$, and that a_1, a_2, a_3, a_4 are distinct. If $k_1 < k_2+k_3+k_4$ (hence Corollary 13.2.6 does not apply) and $k_1+k_4 > k_2+k_3$ (hence Corollary 13.5.3 does not apply either), then

$$I_4 = \frac{\pi}{4}\sum_{j=1}^{4}\sum_{A,B} C_{j,A,B} + \frac{\pi}{2}\prod_{i\neq 1}\frac{\sin(k_i(a_1-a_i))}{a_1-a_i} - \frac{\pi}{2}\sum_{j=2}^{4}\frac{\sin(k_1(a_j-a_1))}{a_j-a_1}\prod_{i\neq 1,j}\frac{\cos(k_i(a_j-a_i))}{a_j-a_i} \tag{13.36}$$

where the summation in the first sum is as in Theorem 13.2.4. Note that the terms $I_{4,j}$ of (13.32) are implicit in (13.36) and may be used to make the case $m = 4$ of Theorem 13.5.1 explicit as has been done in Corollary 13.5.3 for $m = 3$. $\Diamond$

13.6 Conclusions

We present these results for several reasons. First is the intrinsic beauty and utility of the sinc function. It is important in so many areas of computing, approximation theory, and numerical analysis. It is used in interpolation and approximation of functions, approximate evaluation of transforms — e.g., Hilbert, Fourier, Laplace, Hankel, and Mellin transforms as well as the fast Fourier transform — see [Ste93]. It is used in approximating solutions of differential and integral equations, in image processing [Fee10], in other signal processing and in information theory. It is the Fourier transform of the box filter and so central to the understanding of the Gibbs phenomenon [Str81] and its descendants. Much of this is nicely described in [GS90].

Second is that the forensic nature of the mathematics was entertaining. It also made us reflect on how computer packages and databases have changed mathematics over the past forty to fifty years. As our hunt for the history of this MONTHLY problem indicates, better tools for searching our literature are much needed. Finally some of the evaluations merit being better known as they are excellent tests of both computer algebra and numerical integration.

Chapter 14

The p-adic valuation of k-central binomial coefficients

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[SMA09] *The p-adic valuation of k-central binomial coefficients*
(with Tewodros Amdeberhan, Victor H. Moll)
published in Acta Arithmetica, Vol. 140, 2009, p. 31-42

Abstract The coefficients $c(n,k)$ defined by

$$(1-k^2x)^{-1/k} = \sum_{n\geq 0} c(n,k)x^n$$

reduce to the central binomial coefficients $\binom{2n}{n}$ for $k=2$. Motivated by a question of H. Montgomery and H. Shapiro for the case $k=3$, we prove that $c(n,k)$ are integers and study their divisibility properties.

14.1 Introduction

In a recent issue of the American Mathematical Monthly, Hugh Montgomery and Harold S. Shapiro proposed the following problem (Problem 11380, August-September 2008):

For $x \in \mathbb{R}$, let

$$\binom{x}{n} = \frac{1}{n!} \prod_{j=0}^{n-1} (x - j). \tag{14.1}$$

For $n \geq 1$, let a_n be the numerator and q_n the denominator of the rational number $\binom{-1/3}{n}$ expressed as a reduced fraction, with $q_n > 0$.

1. Show that q_n is a power of 3.

2. Show that a_n is odd if and only if n is a sum of distinct powers of 4.

Our approach to this problem employs Legendre's remarkable expression [Leg30]:

$$\nu_p(n!) = \frac{n - s_p(n)}{p - 1}, \tag{14.2}$$

that relates the p-adic valuation of factorials to the sum of digits of n in base p. For $m \in \mathbb{N}$ and a prime p, the p-adic valuation of m, denoted by $\nu_p(m)$, is the highest power of p that divides m. The expansion of $m \in \mathbb{N}$ in base p is written as

$$m = a_0 + a_1 p + \cdots + a_d p^d, \tag{14.3}$$

with integers $0 \leq a_j \leq p - 1$ and $a_d \neq 0$. The function s_p in (14.2) is defined by

$$s_p(m) := a_0 + a_1 + \cdots + a_d. \tag{14.4}$$

Since, for $n > 1$, $\nu_p(n) = \nu_p(n!) - \nu_p((n-1)!)$, it follows from (14.2) that

$$\nu_p(n) = \frac{1 + s_p(n-1) - s_p(n)}{p - 1}. \tag{14.5}$$

The p-adic valuations of binomial coefficients can be expressed in terms of the function s_p:

$$\nu_p\left(\binom{n}{k}\right) = \frac{s_p(k) + s_p(n-k) - s_p(n)}{p - 1}. \tag{14.6}$$

In particular, for the central binomial coefficients $C_n := \binom{2n}{n}$ and $p = 2$, we have

$$\nu_2\left(C_n\right) = 2s_2(n) - s_2(2n) = s_2(n). \tag{14.7}$$

Therefore, C_n is always even and $\frac{1}{2}C_n$ is odd precisely whenever n is a power of 2. This is a well-known result.

The central binomial coefficients C_n have the generating function

$$(1-4x)^{-1/2} = \sum_{n\geq 0} C_n x^n. \tag{14.8}$$

The binomial theorem shows that the numbers in the Montgomery-Shapiro problem bear a similar generating function

$$(1-9x)^{-1/3} = \sum_{n\geq 0} \binom{-\frac{1}{3}}{n} (-9x)^n. \tag{14.9}$$

It is natural to consider the coeffients $c(n,k)$ defined by

$$(1-k^2x)^{-1/k} = \sum_{n\geq 0} c(n,k)x^n, \tag{14.10}$$

which include the central binomial coefficients as a special case. We call $c(n,k)$ the *k-central binomial coefficients*. The expression

$$c(n,k) = (-1)^n \binom{-\frac{1}{k}}{n} k^{2n} \tag{14.11}$$

comes directly from the binomial theorem. Thus, the Montgomery-Shapiro question from (14.1) deals with arithmetic properties of

$$\binom{-\frac{1}{3}}{n} = (-1)^n \frac{c(n,3)}{3^{2n}}. \tag{14.12}$$

14.2 The integrality of $c(n,k)$

It is a simple matter to verify that the coefficients $c(n,k)$ are rational numbers. The expression produced in the next proposition is then employed to prove that $c(n,k)$ are actually integers. The next section will explore divisibility properties of the integers $c(n,k)$.

Proposition 14.2.1. *The coefficient $c(n,k)$ is given by*

$$c(n,k) = \frac{k^n}{n!} \prod_{m=1}^{n-1} (1+km). \tag{14.13}$$

Proof. The binomial theorem yields

$$\begin{aligned}(1-k^2x)^{-1/k} &= \sum_{n\geq 0} \binom{-\frac{1}{k}}{n} (-k^2x)^n \\ &= \sum_{n\geq 0} \frac{k^n}{n!} \left(\prod_{m=1}^{n-1} (1+km) \right) x^n,\end{aligned}$$

and (14.13) has been established. □

An alternative proof of the previous result is obtained from the simple recurrence

$$c(n+1,k) = \frac{k(1+kn)}{n+1} c(n,k), \qquad \text{for } n \geq 0, \tag{14.14}$$

and its initial condition $c(0,k) = 1$. To prove (14.14), simply differentiate (14.10) to produce

$$k(1-k^2x)^{-1/k-1} = \sum_{n\geq 0} (n+1)c(n+1,k)x^n \tag{14.15}$$

and multiply both sides by $1-k^2x$ to get the result.

Note 14.2.2. The coefficients $c(n,k)$ can be written in terms of the Beta function as

$$c(n,k) = \frac{k^{2n}}{nB(n,1/k)}. \tag{14.16}$$

This expression follows directly by writing the product in (14.13) in terms of the Pochhammer symbol $(a)_n = a(a+1)\cdots(a+n-1)$ and the identity

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}. \tag{14.17}$$

The proof employs only the most elementary properties of the Euler's Gamma and Beta functions. The reader can find details in [BM04]. The conclusion is that we have an integral expression for $c(n,k)$, given by

$$c(n,k)\int_0^1 (1-u^{1/n})^{1/k-1}\,du = k^{2n}. \tag{14.18}$$

It is unclear how to use it to further investigate $c(n,k)$.

In the case $k=2$, we have that $c(n,2) = C_n$ is a positive integer. This result extends to all values of k.

Theorem 14.2.3. *The coefficient $c(n,k)$ is a positive integer.*

Proof. First observe that if p is a prime dividing k, then the product in (14.10) is relatively prime to p. Therefore we need to check that $\nu_p(n!) \leq \nu_p(k^n)$. This is simple:

$$\nu_p(n!) = \frac{n-s_p(n)}{p-1} \leq n \leq \nu_p(k^n). \tag{14.19}$$

Now let p be a prime not dividing k. Clearly,

$$\nu_p(c(n,k)) = \nu_p\left(\prod_{m<n}(1+km)\right) - \nu_p\left(\prod_{m<n}(1+m)\right). \tag{14.20}$$

To prove that $c(n,k)$ is an integer, we compare the p-adic valuations of $1+km$ and $1+m$. Observe that $1+m$ is divisible by p^α if and only if m is of the form $\lambda p^\alpha - 1$. On the other hand, $1+km$ is divisible by p^α precisely when m is of the form $\lambda p^\alpha - i_{p^\alpha}(k)$, where $i_{p^\alpha}(k)$ denotes the inverse of k modulo p^α in the range $1,\ 2,\ \cdots, p^\alpha - 1$. Thus,

$$\nu_p(c(n,k)) = \sum_{\alpha \geq 1} \left\lfloor \tfrac{n+i_{p^\alpha}(k)-1}{p^\alpha} \right\rfloor - \left\lfloor \tfrac{n}{p^\alpha} \right\rfloor. \tag{14.21}$$

The claim now follows from $i_{p^\alpha}(k) \geq 1$. □

Next, Theorem 14.2.3 will be slightly strengthened and an alternative proof be provided.

Theorem 14.2.4. *For $n > 0$, the coefficient $c(n,k)$ is a positive integer divisible by k.*

Proof. Expanding the right hand side of the identity

$$(1-k^2x)^{-1} = \left((1-k^2x)^{-1/k}\right)^k \tag{14.22}$$

by the Cauchy product formula gives

$$\sum_{i_1+\cdots+i_k=m} c(i_1,k)c(i_2,k)\cdots c(i_k,k) = k^{2m}, \tag{14.23}$$

where the multisum runs through all the k-tuples of non-negative integers. Obviously $c(0,k) = 1$ and it is easy to check that $c(1,k) = k$. We proceed by induction on n, so we assume the assertion is valid for $c(1,k)$, $c(2,k), \cdots, c(n-1,k)$. We prove the same is true for $c(n,k)$. To this end, break up (14.23) as

$$kc(n,k) + \sum_{\substack{i_1+\cdots+i_k=n \\ 0 \leq i_j < n}} c(i_1,k)c(i_2,k)\cdots c(i_k,k) = k^{2n}. \tag{14.24}$$

Hence by the induction assumption $kc(n,k)$ is an integer.

To complete the proof, divide (14.24) through by k^2 and rewrite as follows

$$\frac{c(n,k)}{k} = k^{2n-2} - \frac{1}{k^2} \sum_{\substack{i_1+\cdots+i_k=n \\ 0 \leq i_j < n}} c(i_1,k)c(i_2,k)\cdots c(i_k,k). \tag{14.25}$$

The key point is that each summand in (14.25) contains *at least two* terms, each one divisible by k. □

Note 14.2.5. W. Lang [Lan00] has studied the numbers appearing in the generating function

$$c2(l;x) := \frac{1-(1-l^2x)^{1/l}}{lx}, \tag{14.26}$$

that bears close relation to the case $k = -l < 0$ of equation (14.10). The special case $l = 2$ yields the Catalan numbers. The author establishes the integrality of the coefficients in the expansion of $c2$ and other related functions.

14.3 The valuation of $c(n,k)$

We consider now the p-adic valuation of $c(n,k)$. The special case when p divides k is easy, so we deal with it first.

Proposition 14.3.1. *Let p be a prime that divides k. Then*

$$\nu_p(c(n,p)) = \nu_p(k)n - \frac{n - s_p(n)}{p-1}. \tag{14.27}$$

Proof. The p-adic valuation of $c(n,p)$ is given by

$$\nu_p(c(n,p)) = \nu_p(k)n - \nu_p(n!) = \nu_p(k)n - \frac{n-s_p(n)}{p-1}. \tag{14.28}$$

Finally note that $s_p(n) = O(\log n)$. $\square$

Note 14.3.2. For p, $k \neq 2$, we have $\nu_p(c(n,p)) \sim \left(\nu_p(k) - \frac{1}{p-1}\right) n$, as $n \to \infty$.

We now turn attention to the case where p does not divide k. Under this assumption, the congruence $kx \equiv 1 \bmod p^\alpha$ has a solution. Elementary arguments of p-adic analysis can be used to produce a p-adic integer that yields the inverse of k. This construction proceeds as follows: first choose b_0 in the range $\{1, 2, \cdots, p-1\}$ to satisfy $kb_0 \equiv 1 \bmod p$. Next, choose c_1, satisfying $kc_1 \equiv 1 \bmod p^2$ and write it as $c_1 = b_0 + kb_1$ with $0 \leq b_1 \leq p-1$. Proceeding in this manner, we obtain a sequence of integers $\{b_j : j \geq 0\}$, such that $0 \leq b_j \leq p-1$ and the partial sums of the *formal object* $x = b_0 + b_1 p + b_2 p^2 + \cdots$ satisfy

$$k\left(b_0 + b_1 p + \cdots + b_{j-1}p^{j-1}\right) \equiv 1 \bmod p^j. \tag{14.29}$$

This is the standard definition of a p-adic integer and

$$i_{p^\infty}(k) = \sum_{j=0}^{\infty} b_j p^j \tag{14.30}$$

is the inverse of k in the ring of p-adic integers. The reader will find in [Gou97] and [Mur02] information about this topic.

Note 14.3.3. It is convenient to modify the notation in (14.30) and write it as

$$i_{p^\infty}(k) = 1 + \sum_{j=0}^{\infty} b_j p^j \tag{14.31}$$

which is always possible since the first coefficient cannot be zero. The reader is invited to check that, when doing so, the b_j are periodic in j with period the multiplicative order of p in $\mathbb{Z}/k\mathbb{Z}$. Furthermore, the b_j take values amongst $\lfloor p/k \rfloor$, $\lfloor 2p/k \rfloor, \ldots, \lfloor (k-1)p/k \rfloor$. This will be exemplified in the case $k = 3$ later.

The analysis of $\nu_p(c(n,k))$ for those primes p not dividing k begins with a characterization of those indices for which $\nu_p(c(n,k)) = 0$, that is, p does not divide $c(n,k)$. The result is expressed in terms of the expansions of n in base p, written as

$$n = a_0 + a_1 p + a_2 p^2 + \cdots + a_d p^d, \tag{14.32}$$

and the p-adic expansion of the inverse of k as given by (14.31).

Theorem 14.3.4. *Let p be a prime that does not divide k. Then $\nu_p(c(n,k)) = 0$ if and only if $a_j + b_j < p$ for all j in the range $1 \leq j \leq d$.*

Proof. It follows from (14.21) that $c(n,k)$ is not divisible by p precisely when

$$\left\lfloor \tfrac{1}{p^\alpha} \left(n + \textstyle\sum_j b_j p^j \right) \right\rfloor = \left\lfloor \tfrac{n}{p^\alpha} \right\rfloor, \tag{14.33}$$

for all $\alpha \geq 1$, or equivalently, if and only if

$$\sum_{j=0}^{\alpha-1} (a_j + b_j) p^j < p^\alpha, \tag{14.34}$$

for all $\alpha \geq 1$. An inductive argument shows that this is equivalent to the condition $a_j + b_j < p$ for all j. Naturally, the a_j vanish for $j > d$, so it is sufficient to check $a_j + b_j < p$ for all $j \leq d$. $\square$

Corollary 14.3.5. *For all primes $p > k$ and $d \in \mathbb{N}$, we have $\nu_p(c(p^d, k)) = 0$.*

Proof. The coefficients of $n = p^d$ in Theorem 14.3.4 are $a_j = 0$ for $0 \leq j \leq d-1$ and $a_d = 1$. Therefore the restrictions on the coefficients b_j become $b_j < p$ for $0 \leq j \leq d-1$ and $b_d < p-1$. It turns out that $b_j \neq p-1$ for all $j \in \mathbb{N}$. Otherwise, for some $r \in \mathbb{N}$, we have $b_r = p-1$ and the equation

$$k \left(1 + \sum_{j=0}^{r-1} b_j p^j + b_r p^r \right) \equiv k \left(1 + \sum_{j=0}^{r-1} b_j p^j - p^r \right) \equiv 1 \bmod p^{r+1}, \tag{14.35}$$

is impossible in view of

$$-kp^r < k\left(1+\sum_{j=0}^{r-1} b_j p^j - p^r\right) < 0. \tag{14.36}$$

□

Now we return again to the Montgomery-Shapiro question. The identity (14.12) shows that the denominator q_n is a power of 3. We now consider the indices n for which $c(n,3)$ is odd and provide a proof of the second part of their problem.

Corollary 14.3.6. *The coefficient* $c(n,3)$ *is odd precisely when* n *is a sum of distinct powers of* 4.

Proof. The result follows from Theorem 14.3.4 and the explicit formula

$$i_{2^\infty}(3) = 1+\sum_{j=0}^{\infty} 2^{2j+1}, \tag{14.37}$$

for the inverse of 3, so that $b_{2j} = 0$ and $b_{2j+1} = 1$. Therefore, if $c(n,3)$ is odd, the theorem now shows that $a_j = 0$ for j odd, as claimed. □

More generally, the discussion of $\nu_p(c(n,3)) = 0$ is divided according to the residue of p modulo 3. This division is a consequence of the fact that for $p = 3u+1$, we have

$$i_{p^\infty}(3) = 1+2u\sum_{m=0}^{\infty} p^m, \tag{14.38}$$

and for $p = 3u+2$, one computes $p^2 = 3(3u^2+4u+1)+1$, to conclude that

$$i_{p^\infty}(3) = 1+2(3u^2+4u+1)\sum_{m=0}^{\infty} p^{2m} = 1+\sum_{m=0}^{\infty} up^{2m} + (2u+1)p^{2m+1}. \tag{14.39}$$

Theorem 14.3.7. *Let $p \neq 3$ be a prime and $n = a_0 + a_1p + a_2p^2 + \ldots + a_dp^d$ as before. Then p does not divide $c(n, 3)$ if and only if the p-adic digits of n satisfy*

$$a_j < \begin{cases} p/3 & \text{if } j \text{ is odd or } p = 3u+1, \\ 2p/3 & \text{otherwise.} \end{cases} \tag{14.40}$$

For general k we have the following analogous statement.

Theorem 14.3.8. *Let $p = ku + 1$ be a prime. Then p does not divide $c(n, k)$ if and only if the p-adic digits of n are less than p/k.*

Observe that Theorem 14.3.8 implies the following well-known property of the central binomial coefficients: C_n is not divisible by $p \neq 2$ if and only if the p-adic digits of n are less than $p/2$.

Now we return to (14.21) which will be written as

$$\nu_p(c(n,k)) = \sum_{\alpha \geq 0} \left\lfloor \tfrac{1}{p^{\alpha+1}} \textstyle\sum_{m=0}^{\alpha} (a_m + b_m)p^m \right\rfloor. \tag{14.41}$$

From here, we bound

$$\sum_{m=0}^{\alpha} (a_m + b_m)p^m \leq \sum_{m=0}^{\alpha} (2p-2)p^m = 2(p^{\alpha+1} - 1) < 2p^{\alpha+1}. \tag{14.42}$$

Therefore, each summand in (14.41) is either 0 or 1. The p-adic valuation of $c(n, p)$ counts the number of 1's in this sum. This proves the final result.

Theorem 14.3.9. *Let p be a prime that does not divide k. Then, with the previous notation for a_m and b_m, we have that $\nu_p(c(n, k))$ is the number of indices m such that either*

- $a_m + b_m \geq p$ *or*

- *there is* $j \leq m$ *such that* $a_{m-i}+b_{m-i} = p-1$ *for* $0 \leq i \leq j-1$ *and* $a_{m-j}+b_{m-j} \geq p$.

Corollary 14.3.10. *Let* p *be a prime that does not divide* k*, and write* $n = \sum a_m p^m$ *and* $i_{p^\infty}(k) = 1 + \sum b_m p^m$*, as before. Let* v_1 *and* v_2 *be the number of indices* m *such that* $a_m + b_m \geq p$ *and* $a_m + b_m \geq p-1$*, respectively. Then*

$$v_1 \leq \nu_p(c(n,k)) \leq v_2. \tag{14.43}$$

14.4 A q-generalization of $c(n,k)$

A standard procedure to generalize an integer expression is to replace $n \in \mathbb{N}$ by the polynomial

$$[q]_n := \frac{1-q^n}{1-q} = 1 + q + q^2 + \ldots + q^{n-1}. \tag{14.44}$$

The original expression is recovered as the limiting case $q \to 1$. For example, the factorial $n!$ is extended to the polynomial

$$[n]_q! := [n]_q[n-1]_q \ldots [2]_q[1]_q = \prod_{j=1}^{n} \frac{1-q^j}{1-q}. \tag{14.45}$$

The reader will find in [KC02] an introduction to this q-world.

In this spirit we generalize the integers

$$c(n,k) = \frac{k^n}{n!} \prod_{m=0}^{n-1} (km+1) = \prod_{m=1}^{n} \frac{k(k(m-1)+1)}{m}, \tag{14.46}$$

into the q-world as

$$F_{n,k}(q) := \prod_{m=1}^{n} \frac{[km]_q[k(m-1)+1]_q}{[m]_q^2}. \tag{14.47}$$

Note that this expression indeed gives $c(n,k)$ as $q \to 1$. The corresponding extension of Theorem 14.2.3 is stated in the next result. The proof is similar to that given above, so it is left to the curious reader.

Theorem 14.4.1. *The function*

$$F_{n,k}(q) := \prod_{m=1}^{n} \frac{(1-q^{km})(1-q^{k(m-1)+1})}{(1-q^m)^2} \tag{14.48}$$

is a polynomial in q with integer coefficients.

14.5 Future directions

In this final section we discuss some questions related to the integers $c(n,k)$.

A combinatorial interpretation The integers $c(n,2)$ are given by the central binomial coefficients $C_n = \binom{2n}{n}$. These coefficients appear in many counting situations: C_n gives the number of walks of length $2n$ on an infinite linear lattice that begin and end at the origin. Moreover, they provide the exact answer for the elementary sum

$$\sum_{k=0}^{n} \binom{n}{k}^2 = C_n. \tag{14.49}$$

Is it possible to produce similar results for $c(n,k)$, with $k \neq 2$? In particular, what do the numbers $c(n,k)$ count?

A further generalization The polynomial $F_{n,k}(q)$ can be written as

$$F_{n,k}(q) = \frac{(1-q)}{(1-q^{kn+1})} \prod_{m=1}^{n} \frac{(1-q^{km})(1-q^{km+1})}{(1-q^m)^2} \tag{14.50}$$

which suggests the extension

$$G_{n,k}(q,t) := \frac{(1-q)}{(1-tq^{kn})} \prod_{m=1}^{n} \frac{(1-q^{km})(1-tq^{km})}{(1-q^m)^2} \tag{14.51}$$

so that $F_{n,k}(q) = G_{n,k}(q,q)$. Observe that $G_{n,k}(q,t)$ is not always a polynomial. For example,

$$G_{2,1}(q,t) = \frac{1-qt}{1-q^2}. \tag{14.52}$$

On the other hand,

$$G_{1,2}(q,t) = q+1. \tag{14.53}$$

The following functional equation is easy to establish.

Proposition 14.5.1. *The function $G_{n,k}(q,t)$ satisfies*

$$G_{n,k}(q,tq^k) = \frac{(1-q^{kn}t)}{(1-q^k t)} G_{n,k}(q,t). \tag{14.54}$$

The reader is invited to explore its properties. In particular, find minimal conditions on n and k to guarantee that $G_{n,k}(q,t)$ is a polynomial.

Consider now the function

$$H_{n,k,j}(q) := G_{n,k}(q,q^j) \tag{14.55}$$

that extends $F_{n,k}(q) = H_{n,k,1}(q)$. The following statement predicts the situation where $H_{n,k,j}(q)$ is a polynomial.

Problem 14.5.2. *Show that $H_{n,k,j}(q)$ is a polynomial precisely if the indices satisfy $k \equiv 0 \bmod gcd(n,j)$.*

A result of Erdös, Graham, Ruzsa and Strauss In this paper we have explored the conditions on n that result in $\nu_p(c(n,k)) = 0$. Given two distinct primes p and

q, P. Erdös et al. [EGRS75] discuss the existence of indices n for which $\nu_p(C_n) = \nu_q(C_n) = 0$. Recall that by Theorem 14.3.8 such numbers n are characterized by having p-adic digits less than $p/2$ and q-adic digits less than $q/2$. The following result of [EGRS75] proves the existence of infinitely many such n.

Theorem 14.5.3. *Let A, $B \in \mathbb{N}$ such that $A/(p-1) + B/(q-1) \geq 1$. Then there exist infinitely many numbers n with p-adic digits $\leq A$ and q-adic digits $\leq B$.*

This leaves open the question for $k > 2$ whether or not there exist infinitely many numbers n such that $c(n, k)$ is neither divisible by p nor by q. The extension to more than two primes is open even in the case $k = 2$. In particular, a prize of \$1000 has been offered by R. Graham for just showing that there are infinitely many n such that C_n is coprime to $105 = 3 \cdot 5 \cdot 7$. On the other hand, it is conjectured that there are only finitely many indices n such that C_n is not divisible by any of 3, 5, 7 and 11.

Finally, we remark that Erdös et al. conjectured in [EGRS75] that the central binomial coefficients C_n are never squarefree for $n > 4$ which has been proved by Granville and Ramare in [GR96]. Define

$$\tilde{c}(n, k) := \text{Numerator}\left(k^{-n} c(n, k)\right). \tag{14.56}$$

We have *some* empirical evidence which suggests the existence of an index $n_0(k)$, such that $\tilde{c}(n, k)$ is not squarefree for $n \geq n_0(k)$. The value of $n_0(k)$ could be large. For instance

$$\begin{aligned}\tilde{c}(178, 5) \quad = \quad & 10233168474238806048538224953529562250076040177895261 \\ & 58561031939088200683714293748693318575050979745244814 \\ & 76554554334063451753661793539394441141469478114 2\end{aligned}$$

is squarefree, so that $n_0(5) \geq 178$. The numbers $\tilde{c}(n,k)$ present new challeges, even in the case $k = 2$. Recall that $\frac{1}{2}C_n$ is odd if and only if n is a power of 2. Therefore, C_{786} is not squarefree. On the other hand, the complete factorization of C_{786} shows that $\tilde{c}(786, 2)$ is squarefree. We conclude that $n_0(2) \geq 786$.

Chapter 15

Positivity of Szegö's rational function

The contents of this chapter (apart from minor corrections or adaptions) have been published as:

[Str08] *Positivity of Szego's rational function*
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Abstract We consider the problem of deciding whether a given rational function has a power series expansion with all its coefficients positive. Introducing an elementary transformation that preserves such positivity we are able to provide an elementary proof for the positivity of Szegö's function

$$\frac{1}{(1-x)(1-y)+(1-y)(1-z)+(1-z)(1-x)}$$

which has been at the historical root of this subject starting with Szegö. We then demonstrate how to apply the transformation to prove a 4-dimensional generalization of the above function, and close with discussing the set of parameters (a, b) such that

$$\frac{1}{1-(x+y+z)+a(xy+yz+zx)+bxyz}$$

has positive coefficients.

15.1 Introduction

A rational function is called *positive* if all its Taylor coefficients are positive. In 1930 H. Lewy and K. Friedrichs conjectured the positivity of the rational function

$$\frac{1}{(1-x)(1-y)+(1-y)(1-z)+(1-z)(1-x)} = \sum_{k,m,n\geqslant 0} a(k,m,n)x^k y^m z^n. \quad (15.1)$$

The positivity of the $a(k,m,n)$ was proved shortly after by G. Szegö employing heavy machinery in [Sze33], but he remarks himself "die angewendeten Hilfsmittel stehen allerdings in keinem Verhältnis zu der Einfachheit des Satzes"[1]. Motivated by these words, T. Kaluza gave an elementary but technically difficult proof that was published in the very same journal [Kal33]. R. Askey and G. Gasper also proved the above positivity in [AG72] using some of Szegö's observations but avoiding the use of Bessel functions in favour of Legendre polynomials. The problem has also been considered in the recent paper [Kau07] by M. Kauers from the viewpoint of computer algebra, and Kauers establishes the result under the constraint that $k \leqslant 16$ by finding appropriate recurrences. We provide an elementary proof of Szegö's result with the main ingredient being a simple positivity preserving operation in the spirit of [GRZ83], whence we reduce the positivity of the coefficients $a(k,m,n)$ to the positivity of another rational function that is easier to handle. While our proof is indeed elementary, to check that the latter rational function is positive is most conveniently done with the aid of computer algebra.

[1] "the used tools, however, are disproportionate to the simplicity of the statement"

15.2 Positivity preserving operations

The following elementary proposition is closely related to the positivity preserving operations given by J. Gillis, B. Reznick and D. Zeilberger in [GRZ83, Proposition 2].

Proposition 15.2.1. *Fix $n \geqslant 1$. Let $1 \leqslant j \leqslant n$ and suppose that the polynomial $p(x_1, \ldots, x_n)$ is linear in x_j. If $1/p(x_1, \ldots, x_n)$ is positive then so is*

$$T_{j,\lambda}\left(\frac{1}{p(x_1, \ldots, x_n)}\right) := \frac{1}{p(x_1, \ldots, x_n) - \lambda x_j p(x_1, \ldots, x_{j-1}, 0, x_{j+1}, \ldots, x_n)}$$

whenever $\lambda \geqslant 0$. In other words, the operator $T_{j,\lambda}$ as defined above is positivity preserving for $\lambda \geqslant 0$.

Proof. We may assume $j = 1$. Write $p(x_1, \ldots, x_n) = a(x_2, \ldots, x_n) - x_1 b(x_2, \ldots, x_n)$. Since

$$\frac{1}{p} = \frac{1}{a - x_1 b} = \sum_{n \geqslant 0} \frac{b^n}{a^{n+1}} x_1^n$$

has positive coefficients so does b^n/a^{n+1}. The quotient

$$\frac{b^n}{a^{n+1}} \frac{x_1^n}{(1 - \lambda x_1)^{n+1}}$$

has nonnegative coefficients, and for $n = 0$ they are all positive. This finally implies the positivity of

$$\sum_{n \geqslant 0} \frac{(x_1 b)^n}{((1 - \lambda x_1)a)^{n+1}} = \frac{1}{(1 - \lambda x_1)a - x_1 b} = \frac{1}{p - \lambda x_1 a}.$$

□

In this paper, we will only be interested in the positivity of symmetric rational functions $1/p$. We therefore introduce another operator which preserves both positivity and symmetry.

Corollary 15.2.2. *The operator T_λ defined by*

$$T_\lambda := T_{n,\lambda} \cdots T_{2,\lambda} T_{1,\lambda}$$

is positivity preserving for $\lambda \geqslant 0$.

Note that $T_\lambda(1/p)$ is only defined for polynomials p which are linear in each of their variables. Further note that $T_{j,\lambda}$ is invertible with $T_{j,\lambda}^{-1} = T_{j,-\lambda}$. Since the operators $T_{1,\lambda}, T_{2,\lambda}, \ldots, T_{n,\lambda}$ commute, this shows that T_λ is invertible as well and $T_\lambda^{-1} = T_{-\lambda}$. Hence, in order to establish the positivity of $1/p$ it is sufficient to do so for some $T_{-\lambda}(1/p)$ with $\lambda \geqslant 0$. That T_λ preserves symmetry also follows from the fact that $T_{1,\lambda}, \ldots, T_{n,\lambda}$ commute.

Example 15.2.3. To prove positivity of $1/p(x,y,z)$, assuming p to be linear in each of x, y, z, it suffices to prove positivity of

$$T_{-1}\left(\frac{1}{p(x,y,z)}\right) = \begin{array}{c} (p(x,y,z) + xp(0,y,z) + yp(x,0,z) + zp(x,y,0) \\ +xyp(0,0,z) + yzp(x,0,0) + zxp(0,y,0) + xyzp(0,0,0))^{-1} \end{array}$$

Notice that the right-hand side is indeed a symmetric rational function if p is symmetric itself.

15.3 Szegö's rational function

15.3.1 Positivity of Szegö's rational function

Theorem 15.3.1. *Szegö's rational function*

$$f(x,y,z) := \frac{1}{1-2(x+y+z)+3(xy+yz+zx)}$$

is positive.

Remark 15.3.2. Note that up to rescaling this is the rational function from (15.1), namely

$$\frac{1}{3}f\left(\frac{x}{3},\frac{y}{3},\frac{z}{3}\right) = \frac{1}{(1-x)(1-y)+(1-y)(1-z)+(1-z)(1-x)}.$$

Proof. The denominator of f is linear in all the variables x, y, z, so we can apply our inverted positivity preserving operation T_{-1}. We obtain

$$g(x,y,z) := T_{-1}(f(x,y,z)) = \frac{1}{1-(x+y+z)+4xyz}.$$

By Corollary 15.2.2 positivity of g implies positivity of f. The positivity of g, however, is well-known, and several short proofs have been given in the literature (not so, to our knowledge, for f). One possibility is to note that the coefficients $b(k,m,n)$ of g satisfy the following recurrence, first observed by J. Gillis and J. Kleeman [GK79],

$$(1+n)b(k+1,m+1,n+1) = 2(n+m-k)b(k+1,m,n)+(1+n-m+k)b(k+1,m+1,n),$$

which together with the initial $b(0,0,0) = 1$ proves positivity of the $b(k,m,n)$ by induction. That the $b(k,m,n)$ satisfy this recurrence is verified by just checking that their generating function g solves the corresponding differential equation. $\square$

Remark 15.3.3. Kauers describes in [Kau07] how to automatically find positivity proving recurrences with computer algebra, and also remarks that no such first-order recurrence with linear coefficients exists for Szegö's f.

Another simple proof of the positivity of g based on MacMahon's master theorem is given by M. Ismail and M. Tamhankar in [IT79]. We will discuss this theorem in Section 15.3.3. The reason for doing so is that we discovered the transformation presented in Corollary 15.2.2 by applying MacMahon's master theorem, whence it is possible to just *see* its impact.

15.3.2 A 4-dimensional generalization

Following [Sze33, §3] we define

$$q_n(t) = \prod_{k=1}^{n} (t - x_k),$$

and observe that one can recover Szegö's function as

$$\frac{1}{q_3'(1)} = \frac{1}{(1-x_1)(1-x_2) + (1-x_2)(1-x_3) + (1-x_3)(1-x_1)}.$$

Szegö proves that $1/q_n'(1)$ as a rational function in $x_1, \ldots, x_n$ has positive Taylor coefficients for all $n \geqslant 2$, and remarks that the essential difficulty lies in the cases $n = 3$ and $n = 4$. While our previous discussion covers $n = 3$, we now want to briefly demonstrate how to use the operators T_λ from Corollary 15.2.2 to also establish the case $n = 4$ in an elementary way.

Theorem 15.3.4. *The rational function*

$$\frac{1}{q_4'(1)} = \frac{1}{\sum_{i<j<k} (1-x_i)(1-x_j)(1-x_k)},$$

where $i, j, k = 1, 2, 3, 4,$ is positive.

Proof. Expanding the denominator of $1/q_4'(1)$ and rescaling produces the rational function

$$\frac{1}{1 - 3\sum_i x_i + 8\sum_{i<j} x_i x_j - 16\sum_{i<j<k} x_i x_j x_k}.$$

Applying T_{-2} we find that it suffices to establish positivity of

$$\frac{1}{1 - \sum_i x_i + 4\sum_{i<j<k} x_i x_j x_k - 16 x_1 x_2 x_3 x_4}.$$

This again is a well-known result. In particular, Gillis, Reznick and Zeilberger demonstrate in [GRZ83] how a single application of their elementary methods can be used to deduce the desired positivity. □

For other possible generalizations of Szegö's function the interested reader is referred to [AG72], [Ask74]. In [AIK78] relations to rearrangement problems and integrals of products of Laguerre polynomials are studied.

15.3.3 MacMahon's master theorem

The following is a celebrated result of P. A. MacMahon published in [Mac15], and coined by himself as "a master theorem in the Theory of Permutations".

Theorem 15.3.5 (MacMahon, 1915)**.** *Let R be a commutative ring, $A \in R^{n\times n}$ a matrix, and $x = (x_1, \ldots, x_n)$ commuting indeterminants. For every multi-index $m = (m_1, \ldots, m_n) \in \mathbb{Z}_{\geqslant 0}^n$*

$$[x^m] \prod_{i=1}^n \left(\sum_{j=1}^n A_{i,j} x_i \right)^{m_i} = [x^m] \det \left(I_n - A \begin{pmatrix} x_1 & & \\ & \ddots & \\ & & x_n \end{pmatrix} \right)^{-1},$$

where $[x^m]$ *denotes the coefficient of* $x_1^{m_1} \cdots x_n^{m_n}$ *in the expansion of what follows.*

We find, preferably by using computer algebra, that Szegö's function $f(x, y, z)$ can be expressed as

$$\frac{1}{1 - 2(x + y + z) + 3(xy + yz + zx)} = \det \left(I_3 - \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix} \begin{pmatrix} x & & \\ & y & \\ & & z \end{pmatrix} \right)^{-1}.$$

MacMahon's theorem 15.3.5 now asserts that the coefficient $a(k, m, n)$ of $x^k y^m z^n$ in this expansion is equal to the coefficient of $x^k y^m z^n$ in

$$(2x - y - z)^k (-x + 2y - z)^m (-x - y + 2z)^n.$$

Using the binomial theorem this product is equal to

$$\sum_{r,s,t} \binom{k}{r} \binom{m}{s} \binom{n}{t} x^{k-r} y^{m-s} z^{n-t} (x - y - z)^r (-x + y - z)^s (-x - y + z)^t,$$

which shows that in order to establish positivity of the $a(k, m, n)$ it is sufficient to prove positivity of the coefficient of $x^r y^s z^t$ in

$$(x - y - z)^r (-x + y - z)^s (-x - y + z)^t.$$

By applying MacMahon's master theorem 15.3.5 backwards we find that

$$\det \left(I_3 - \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} x & & \\ & y & \\ & & z \end{pmatrix} \right)^{-1} = \frac{1}{1 - (x + y + z) + 4xyz},$$

which once more reduces positivity of f to the positivity of g.

With this example in mind, we see the following relation to the positivity preserving operations T_λ: Let f be a rational function that T_λ can be applied to and which can be represented as $f = 1/\det(I - AX)$ for some matrix A (here X denotes the diagonal matrix with the variables of f as its entries). Then $T_\lambda(f) = 1/\det(I - A_\lambda X)$ where A_λ is obtained from A by increasing all its diagonal entries by λ. Similarly, application of $T_{j,\lambda}$ corresponds to increasing the j-th diagonal element by λ. Thus when working with a matrix A corresponding to f instead of with f itself, the action of the positivity preserving operators described here is plainly visible.

15.4 On positivity of a family of rational functions

Kauers states that "it is easy to show that there can be no algorithm which for a given multivariate rational function decides whether all its series coefficients are positive", see [Kau07]. Therefore we focus on the reciprocals of certain symmetric polynomials. In the 3-dimensional case we have the 4 elementary symmetric polynomials

$$1, \qquad x + y + z, \qquad xy + yz + zx, \qquad xyz,$$

and if we further require that every variable appears at most linearly, the most general normalized candidate for positivity is

$$h_{a,b}(x, y, z) = \frac{1}{1 - (x + y + z) + a(xy + yz + zx) + bxyz}.$$

We are interested in the set of all (a, b) such that $h_{a,b}$ has positive coefficients. First, we note that positivity of some $h_{a,b}$ implies positivity of $h_{a',b'}$ whenever $a' \leqslant a$ and $b' \leqslant b$. This is a consequence of the following general fact.

Proposition 15.4.1. *Let $1/p(x_1, \ldots, x_r)$ be a positive rational function, and $q(x_1, \ldots, x_r)$ any polynomial with non-negative coefficients. Then the rational function*

$$\frac{1}{p-q}$$

is positive provided that it has no pole at the origin.

Proof. This follows from the geometric summation

$$\frac{1}{p-q} = \frac{1}{p} \sum_{n \geqslant 0} \left(\frac{q}{p} \right)^n .$$

□

Example 15.4.2. We shortly demonstrate another application of this fact. In [Kau07], it was conjectured that the rational function

$$\frac{1}{1-(x+y+z)+\frac{1}{4}(x^2+y^2+z^2)}$$

is positive. Clearly,

$$\frac{1}{(1-x)^2}$$

has positive coefficents, and thus has

$$\frac{1}{(1-\frac{x+y+z}{2})^2} = \frac{1}{1-(x+y+z)+\frac{1}{2}(xy+yz+zx)+\frac{1}{4}(x^2+y^2+z^2)}.$$

Proposition 15.4.1 now implies positivity of the function considered by Kauers.

Based upon numerical evidence and partial proofs, which will be provided in the sequel, we present the following conjecture attempting to describe the set of all (a, b) such that $h_{a,b}$ has positive coefficients.

Conjecture 15.4.3. *The rational function $h_{a,b}$ has positive coefficients if and only if*

$$\begin{cases} b < 6(1-a) \\ b \leqslant 2 - 3a + 2(1-a)^{3/2} \\ a \leqslant 1 \end{cases}.$$

Figure 15.1 shows the region defined by the restrictions given in Conjecture 15.4.3 with the points corresponding to Szegö's function $f(x,y,z) = h_{3/4,0}(2x,2y,2z)$ and $g = h_{0,4}$ marked.

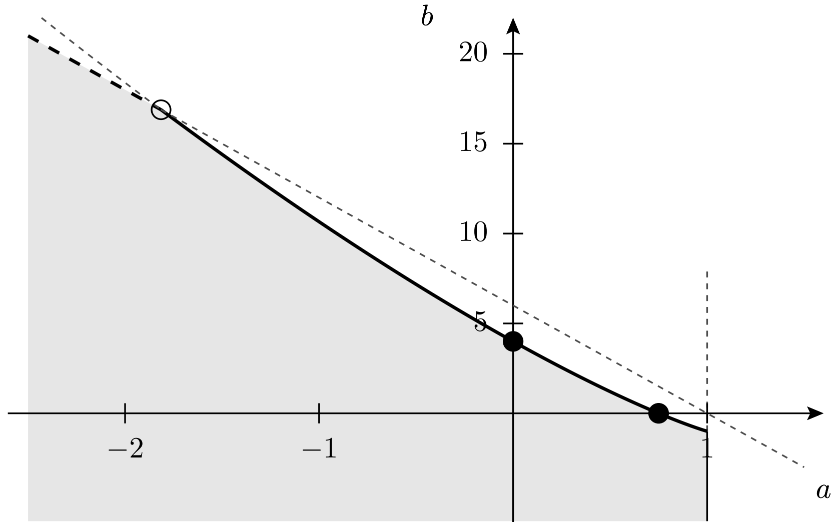

Figure 15.1: Region of Positivity of $h_{a,b}$

First, we turn to the "if" part of Conjecture 15.4.3, that is conditions for the (a,b) that are sufficient for positivity of $h_{a,b}$.

Proposition 15.4.4. *$h_{a,b}$ is positive if $0 \leqslant a \leqslant 1$ and $b \leqslant 2 - 3a + 2(1-a)^{3/2}$.*

Proof. Let $\lambda \geqslant 0$. By Corollary 15.2.2 positivity of some $h_{a,b}$ implies positivity of $h_{a',b'} := T_\lambda(h_{a,b})$ (here we mean that $h_{a',b'}$ equals $T_\lambda(h_{a,b})$ up to rescaling the variables), where

$$a' = \frac{a + 2\lambda + \lambda^2}{(1+\lambda)^2}, \quad b' = \frac{b - 3\lambda a - 3\lambda^2 - \lambda^3}{(1+\lambda)^3}.$$

Starting with the positivity of $g = h_{0,4}$, that is $(a, b) = (0, 4)$, we find that $b' = 2 - 3a' + 2(1 - a')^{3/2}$. Using Proposition 15.4.1 this proves the case $0 \leqslant a < 1$. For $a = 1$ observe that

$$h_{1,-1}(x, y, z) = \frac{1}{(1 - x)(1 - y)(1 - z)}$$

is obviously positive. □

Using the positivity of g and the positivity preserving operations T_λ we have thus been able to prove the "if" part of Conjecture 15.4.3 under the hypothesis that $a \geqslant 0$. Clearly, we can strengthen this hypothesis to $a \geqslant a_1$ if we succeed in proving the positivity of h_{a_1,b_1} with $b_1 = 2 - 3a_1 + 2(1 - a_1)^{3/2}$. However, according to Conjecture 15.4.3 we neccessarily have $a_1 > a_0$, where $a_0 \approx -1.81451$ is the unique real solution of

$$2 - 3a_0 + 2(1 - a_0)^{3/2} = 6(1 - a_0).$$

Let's now consider the "only if" direction of Conjecture 15.4.3.

Proposition 15.4.5. *$h_{a,b}$ is positive only if $b < 6(1 - a)$ and $a \leqslant 1$.*

Proof. Observe that the coefficient of xyz in the expansion of $h_{a,b}(x, y, z)$ evaluates as $6(1 - a) - b$ which proves that $b < 6(1 - a)$ for positivity.

For the second claim we expand $h_{a,b}(x, y, 0)$ as

$$h_{a,b}(x, y, 0) = \frac{1}{1 - x - y + axy} = \sum_{n \geqslant 0} \frac{(1 - ax)^n}{(1 - x)^{n+1}} y^n.$$

Using

$$\frac{1}{(1 - x)^{n+1}} = \sum_{m \geqslant 0} \binom{n + m}{n} x^m,$$

we deduce that the coefficient of xy^n in $h_{a,b}(x, y, z)$ is given by $n + 1 - na$. Positivity of $h_{a,b}$ thus implies that

$$a < \frac{n + 1}{n}$$

for all positive integers n. $\square$

Proposition 15.4.4 is based upon the positivity of $g = h_{0,4}$, which by Proposition 15.4.1 implies that $b \leqslant 4$ suffices for positivity of $h_{0,b}$. This bound turns out to be sharp.

Proposition 15.4.6. *$h_{0,b}$ is positive only if $b \leqslant 4$.*

Proof. We expand $h_{0,b}$ as

$$h_{0,b}(x,y,z) = \frac{1}{1-x-y-z+bxyz} = \sum_{n \geqslant 0} \frac{(1-bxy)^n}{(1-x-y)^{n+1}} z^n.$$

Using

$$\frac{1}{(1-x-y)^{n+1}} = \sum_{m \geqslant 0} \binom{n+m}{n} (x+y)^m,$$

we conclude that the coefficient of $xy^n z^n$ in $h_{0,b}(x,y,z)$ is given by

$$(n+1)\binom{2n+1}{n} - bn\binom{2n-1}{n}.$$

Positivity of $h_{0,b}$ then implies that

$$b < \frac{2(2n+1)}{n}$$

for all integers $n > 0$. $\square$

Corollary 15.4.7. *Let $a \leqslant 0$. Then $h_{a,b}$ is positive only if $b \leqslant 2 - 3a + 2(1-a)^{3/2}$.*

Proof. Otherwise an application of T_λ with appropriate $\lambda > 0$ would produce (after normalization) a positive $h_{0,b'}$ with $b' > 4$ contradicting Proposition 15.4.6. $\square$

To improve on the hypothesis $a \leqslant 0$, it would be desirable to show optimality of Szegö's function, that is that $h_{a,0}$ is positive only if $a \leqslant 3/4$. As in the proof of

Proposition 15.4.6 we believe that it suffices to consider the coefficients of xy^nz^n in $h_{a,0}(x,y,z)$. While we readily find a second order recurrence for those coefficients we didn't see how to derive the necessity of $a \leqslant 3/4$ in order to prove positivity.

Example 15.4.8. By computing the first 100 coefficients of xy^nz^n in $h_{a,0}(x,y,z)$ we learn that $h_{a,0}$ is positive only if $a < 0.75188$.

The (conjectured) optimality of Szegö's function f is surprising in this context since $f = T_1(g)$ allows us to conclude the positivity of f from the positivity of g but not vice versa. Yet, the positivity preserving operator T_1 still provided us with an optimal result. In fact, more seems to be true. As stated in Conjecture 15.4.3, starting with a positive $h_{a,b}$ which is optimal (in the sense that increasing either a or b will destroy positivity) the positivity preserving operators T_λ, $\lambda \geqslant 0$, not only yield a positive rational function $T_\lambda(h_{a,b})$ but again they seem to produce an optimal rational function.

Chapter 16

A q-analog of Ljunggren's binomial congruence

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Abstract We prove a q-analog of a classical binomial congruence due to Ljunggren which states that

$$\binom{ap}{bp} \equiv \binom{a}{b}$$

modulo p^3 for primes $p \geqslant 5$. This congruence subsumes and builds on earlier congruences by Babbage, Wolstenholme and Glaisher for which we recall existing q-analogs. Our congruence generalizes an earlier result of Clark.

16.1 Introduction and notation

Recently, q-analogs of classical congruences have been studied by several authors including [Cla95], [And99], [SP07], [Pan07], [CP08], [Dil08]. Here, we consider the classical congruence

$$\binom{ap}{bp} \equiv \binom{a}{b} \mod p^3 \tag{16.1}$$

which holds true for primes $p \geqslant 5$. This also appears as Problem 1.6 (d) in [Sta97]. Congruence (16.1) was proved in 1952 by Ljunggren, see [Gra97], and subsequently generalized by Jacobsthal, see Remark 16.4.2.

Let $[n]_q := 1 + q + \ldots q^{n-1}$, $[n]_q! := [n]_q[n-1]_q \cdots [1]_q$ and

$$\binom{n}{k}_q := \frac{[n]_q!}{[k]_q![n-k]_q!}$$

denote the usual q-analogs of numbers, factorials and binomial coefficients respectively. Observe that $[n]_1 = n$ so that in the case $q = 1$ we recover the usual factorials and binomial coefficients as well. Also, recall that the q-binomial coefficients are polynomials in q with nonnegative integer coefficients. An introduction to these q-analogs can be found in [Sta97].

We establish the following q-analog of (16.1):

Theorem 16.1.1. *For primes $p \geqslant 5$ and nonnegative integers a, b,*

$$\binom{ap}{bp}_q \equiv \binom{a}{b}_{q^{p^2}} - \binom{a}{b+1}\binom{b+1}{2}\frac{p^2-1}{12}(q^p-1)^2 \mod [p]_q^3. \tag{16.2}$$

The congruence (16.2) and similar ones to follow are to be understood over the ring of polynomials in q with integer coefficients. We remark that $p^2 - 1$ is divisible by 12 for all primes $p \geqslant 5$.

Observe that (16.2) is indeed a q-analog of (16.1): as $q \to 1$ we recover (16.1).

Example 16.1.2. Choosing $p = 13$, $a = 2$, and $b = 1$, we have

$$\binom{26}{13}_q = 1 + q^{169} - 14(q^{13}-1)^2 + (1 + q + \ldots + q^{12})^3 f(q)$$

where $f(q) = 14 - 41q + 41q^2 - \ldots + q^{132}$ is an irreducible polynomial with integer coefficients. Upon setting $q = 1$, we obtain $\binom{26}{13} \equiv 2$ modulo 13^3.

Since our treatment very much parallels the classical case, we give a brief history of the congruence (16.1) in the next section before turning to the proof of Theorem 16.1.1.

16.2 A bit of history

A classical result of Wilson states that $(n-1)!+1$ is divisible by n if and only if n is a prime number. "In attempting to discover some analogous expression which should be divisible by n^2, whenever n is a prime, but not divisible if n is a composite number", [Bab19], Babbage is led to the congruence

$$\binom{2p-1}{p-1} \equiv 1 \mod p^2 \tag{16.3}$$

for primes $p \geqslant 3$. In 1862 Wolstenholme, [Wol62], discovered (16.3) to hold modulo p^3, "for several cases, in testing numerically a result of certain investigations, and after some trouble succeeded in proving it to hold universally" for $p \geqslant 5$. To this end, he proves the fractional congruences

$$\sum_{i=1}^{p-1} \frac{1}{i} \equiv 0 \mod p^2, \tag{16.4}$$

$$\sum_{i=1}^{p-1} \frac{1}{i^2} \equiv 0 \mod p \tag{16.5}$$

for primes $p \geqslant 5$. Using (16.4) and (16.5) he then extends Babbage's congruence (16.3) to hold modulo p^3:

$$\binom{2p-1}{p-1} \equiv 1 \mod p^3 \tag{16.6}$$

for all primes $p \geqslant 5$. Note that (16.6) can be rewritten as $\binom{2p}{p} \equiv 2$ modulo p^3. The further generalization of (16.6) to (16.1), according to [Gra97], was found by

Ljunggren in 1952. The case $b = 1$ of (16.1) was obtained by Glaisher, [Gla00], in 1900.

In fact, Wolstenholme's congruence (16.6) is central to the further generalization (16.1). This is just as true when considering the q-analogs of these congruences as we will see here in Lemma 16.4.1.

A q-analog of the congruence of Babbage has been found by Clark [Cla95] who proved that

$$\binom{ap}{bp}_q \equiv \binom{a}{b}_{q^{p^2}} \mod [p]_q^2. \tag{16.7}$$

We generalize this congruence to obtain the q-analog (16.2) of Ljunggren's congruence (16.1). A result similar to (16.7) has also been given by Andrews in [And99].

Our proof of the q-analog proceeds very closely to the history just outlined. Besides the q-analog (16.7) of Babbage's congruence (16.3) we will employ q-analogs of Wolstenholme's harmonic congruences (16.4) and (16.5) which were recently supplied by Shi and Pan, [SP07]:

Theorem 16.2.1. *For primes $p \geqslant 5$,*

$$\sum_{i=1}^{p-1} \frac{1}{[i]_q} \equiv -\frac{p-1}{2}(q-1) + \frac{p^2-1}{24}(q-1)^2[p]_q \mod [p]_q^2 \tag{16.8}$$

as well as

$$\sum_{i=1}^{p-1} \frac{1}{[i]_q^2} \equiv -\frac{(p-1)(p-5)}{12}(q-1)^2 \mod [p]_q. \tag{16.9}$$

This generalizes an earlier result [And99] of Andrews.

16.3 A q-analog of Ljunggren's congruence

In the classical case, the typical proof of Ljunggren's congruence (16.1) starts with the Chu-Vandermonde identity which has the following well-known q-analog:

Theorem 16.3.1.

$$\binom{m+n}{k}_q = \sum_j \binom{m}{j}_q \binom{n}{k-j}_q q^{j(n-k+j)}.$$

We are now in a position to prove the q-analog of (16.1).

Proof of Theorem 16.1.1. As in [Cla95] we start with the identity

$$\binom{ap}{bp}_q = \sum_{c_1+\ldots+c_a=bp} \binom{p}{c_1}_q \binom{p}{c_2}_q \cdots \binom{p}{c_a}_q q^{p\sum_{1\leqslant i\leqslant a}(i-1)c_i - \sum_{1\leqslant i<j\leqslant a} c_i c_j} \tag{16.10}$$

which follows inductively from the q-analog of the Chu-Vandermonde identity given in Theorem 16.3.1. The summands which are not divisible by $[p]_q^2$ correspond to the c_i taking only the values 0 and p. Since each such summand is determined by the indices $1 \leqslant j_1 < j_2 < \ldots < j_b \leqslant a$ for which $c_i = p$, the total contribution of these terms is

$$\sum_{1\leqslant j_1<\ldots<j_b\leqslant a} q^{p^2\sum_{k=1}^{b}(j_k-1)-p^2\binom{b}{2}} = \sum_{0\leqslant i_1\leqslant\ldots\leqslant i_b\leqslant a-b} q^{p^2\sum_{k=1}^{b} i_k} = \binom{a}{b}_{q^{p^2}}.$$

This completes the proof of (16.7) given in [Cla95].

To obtain (16.2) we now consider those summands in (16.10) which are divisible by $[p]_q^2$ but not divisible by $[p]_q^3$. These correspond to all but two of the c_i taking values 0 or p. More precisely, such a summand is determined by indices $1 \leqslant j_1 < j_2 < \ldots < j_b < j_{b+1} \leqslant a$, two subindices $1 \leqslant k < \ell \leqslant b+1$, and $1 \leqslant d \leqslant p-1$ such that

$$c_i = \begin{cases} d \text{ for } i = j_k, \\ p-d \text{ for } i = j_\ell, \\ p \text{ for } i \in \{j_1, \ldots, j_{b+1}\} \backslash \{j_k, j_\ell\}, \\ 0 \text{ for } i \notin \{j_1, \ldots, j_{b+1}\}. \end{cases}$$

For each fixed choice of the j_i and k, ℓ the contribution of the corresponding summands is

$$\sum_{d=1}^{p-1} \binom{p}{d}_q \binom{p}{p-d}_q q^{p\sum_{1\leqslant i\leqslant a}(i-1)c_i - \sum_{1\leqslant i<j\leqslant a} c_i c_j}$$

which, using that $q^p \equiv 1$ modulo $[p]_q$, reduces modulo $[p]_q^3$ to

$$\sum_{d=1}^{p-1} \binom{p}{d}_q \binom{p}{p-d}_q q^{d^2} = \binom{2p}{p}_q - [2]_{q^{p^2}}.$$

We conclude that

$$\binom{ap}{bp}_q \equiv \binom{a}{b}_{q^{p^2}} + \binom{a}{b+1}\binom{b+1}{2}\left(\binom{2p}{p}_q - [2]_{q^{p^2}}\right) \mod [p]_q^3. \tag{16.11}$$

The general result therefore follows from the special case $a = 2$, $b = 1$ which is separately proved next. □

16.4 A q-analog of Wolstenholme's congruence

We have thus shown that, as in the classical case, the congruence (16.2) can be reduced, via (16.11), to the case $a = 2$, $b = 1$. The next result therefore is a q-analog of Wolstenholme's congruence (16.6).

Lemma 16.4.1. *For primes $p \geqslant 5$,*

$$\binom{2p}{p}_q \equiv [2]_{q^{p^2}} - \frac{p^2-1}{12}(q^p-1)^2 \mod [p]_q^3.$$

Proof. Using that $[an]_q = [a]_{q^n}[n]_q$ and $[n+m]_q = [n]_q + q^n [m]_q$ we compute

$$\binom{2p}{p}_q = \frac{[2p]_q [2p-1]_q \cdots [p+1]_q}{[p]_q [p-1]_q \cdots [1]_q} = \frac{[2]_{q^p}}{[p-1]_q!} \prod_{k=1}^{p-1}\left([p]_q + q^p [p-k]_q\right)$$

which modulo $[p]_q^3$ reduces to (note that $[p-1]_q!$ is relatively prime to $[p]_q^3$)

$$[2]_{q^p}\left(q^{(p-1)p}+q^{(p-2)p}\sum_{1\leqslant i\leqslant p-1}\frac{[p]_q}{[i]_q}+q^{(p-3)p}\sum_{1\leqslant i<j\leqslant p-1}\frac{[p]_q\,[p]_q}{[i]_q\,[j]_q}\right). \tag{16.12}$$

Combining the results (16.8) and (16.9) of Shi and Pan, [SP07], given in Theorem 16.2.1, we deduce that for primes $p\geqslant 5$,

$$\sum_{1\leqslant i<j\leqslant p-1}\frac{1}{[i]_q\,[j]_q}\equiv\frac{(p-1)(p-2)}{6}(q-1)^2 \mod [p]_q. \tag{16.13}$$

Together with (16.8) this allows us to rewrite (16.12) modulo $[p]_q^3$ as

$$[2]_{q^p}\left(q^{(p-1)p}+q^{(p-2)p}\left(-\frac{p-1}{2}(q^p-1)+\frac{p^2-1}{24}(q^p-1)^2\right)+\right.$$
$$\left.+q^{(p-3)p}\frac{(p-1)(p-2)}{6}(q^p-1)^2\right).$$

Using the binomial expansion

$$q^{mp}=((q^p-1)+1)^m=\sum_k\binom{m}{k}(q^p-1)^k$$

to reduce the terms q^{mp} as well as $[2]_{q^p}=1+q^p$ modulo the appropriate power of $[p]_q$ we obtain

$$\binom{2p}{p}_q\equiv 2+p(q^p-1)+\frac{(p-1)(5p-1)}{12}(q^p-1)^2 \mod [p]_q^3.$$

Since

$$[2]_{q^{p^2}}\equiv 2+p(q^p-1)+\frac{(p-1)p}{2}(q^p-1)^2 \mod [p]_q^3$$

the result follows. □

Remark 16.4.2. Jacobsthal, see [Gra97], generalized the congruence (16.1) to hold modulo p^{3+r} where r is the p-adic valuation of

$$ab(a-b)\binom{a}{b} = 2a\binom{a}{b+1}\binom{b+1}{2}.$$

It would be interesting to see if this generalization has a nice analog in the q-world.

Chapter 17

Outlook

In the following two final sections we comment on certain aspects of two methods which have been in repeated use throughout this thesis: the method of brackets and the method of creative telescoping. We demonstrate how, at least in each particular instance, the method of brackets can be made rigorous by translating its application into the framework of Mellin–Barnes contour integrals. Finally we describe a situaton in which a direct application of creative telescoping is prevented by the divergence of the involved integrals. It is pointed out that, on the level of Mellin calculus, the difficulties at hand can be dealt with by considering distributions instead of classical functions. For both methods this indicates opportunities for further investigation.

17.1 The method of brackets and similar approaches

The method of brackets has been discussed in Chapters 8 and 9. In particular, it was shown that it can be regarded as a multi-dimensional extension of Ramanujan's Master Theorem in the form

$$\int_0^\infty x^{s-1} \left[\sum_{n=0}^\infty \frac{(-1)^n}{n!} \lambda(n) x^n \right] \mathrm{d}x = \Gamma(s)\lambda(-s). \tag{17.1}$$

In Section 17.1.1 below, we briefly sketch the negative dimensional integration (NDIM) approach [HR87] which led [GS07] to the method of brackets, initially referred to as optimized NDIM. While the fundamental (formal) objects in NDIM are the integrals

$$\int_{-\infty}^{\infty} (x^2)^{\alpha} \, \mathrm{d}^D x,$$

a very natural choice in the context of the evaluation of Feynman integrals, the method of brackets revolves around the (formal) integrals

$$\int_{0}^{\infty} x^{\alpha-1} \, \mathrm{d}x,$$

which are usually more convenient for the evaluation of general definite integrals as collected, for instance, in [GR80].

In Section 17.1.2 we describe, mostly by example, how an application of the method of brackets can be made rigorous by writing the integrand in terms of Mellin–Barnes contour integrals which is a common practice in the context of evaluating Feynman integrals [Smi06]. The heuristic part of the method of brackets is Rule 8.9.3 which postulates that an integral is evaluated as the joint contribution of the summations (each corresponding to a choice of free variables) converging in a common region. As will become clear, this situation corresponds to a representation of the desired integral as a multiple Mellin–Barnes integral: closing the contours in a particular way and collecting the appropriate residues yields a series which gives the integral in its region of convergence. For future investigations, it would be interesting to make the relation between combinations of free variables and collections of residues more explicit. Further, given a multiple Mellin–Barnes integral

$$\frac{1}{(2\pi i)^n} \int_{c_1 - i\infty}^{c_1 + i\infty} \cdots \int_{c_n - i\infty}^{c_n + i\infty} \frac{\prod_{k=1}^{r} \Gamma(L_k(s_1, \ldots, s_n))}{\prod_{k=r+1}^{s} \Gamma(L_k(s_1, \ldots, s_n))} x_1^{-s_1} \cdots x_n^{-s_n} \, \mathrm{d}s_1 \cdots \mathrm{d}s_n, \quad (17.2)$$

where the L_k are affine, it would be useful to have a systematic way of determining appropriate sets of residues whose sum represents (17.2) in a chosen region. For $n = 2$ this problem is discussed in [FG12].

17.1.1 Negative dimensional integration

In the negative dimensional integration (NDIM) approach, advocated in [HR87], one makes the formal definition

$$\int_{-\infty}^{\infty} (x^2)^{\alpha}\,\mathrm{d}^D x = (-1)^{\alpha}\pi^{D/2}\Gamma(\alpha+1)\;\delta_{\alpha+D/2,0}. \tag{17.3}$$

Here, $x = (x_1, \ldots, x_D)$, $x^2 = x_1^2 + \ldots + x_D^2$ and $\delta_{i,j}$ is the Kronecker delta. This formal identity is used for nonnegative α and gives a non-zero value only when the $D \leqslant 0$, which explains the label of negative dimensionality.

Initially, α is a positive integer and the definition (17.3) is motivated by taking the limit $\beta \to 0$ of

$$\int_{-\infty}^{\infty} \frac{(x^2)^{\alpha}}{(x^2+M^2)^{\beta}}\,\mathrm{d}^D x = \pi^{D/2}(M^2)^{D/2+\alpha-\beta}\frac{\Gamma(\alpha+D/2)\Gamma(\beta-\alpha-D/2)}{\Gamma(D/2)\Gamma(\beta)}. \tag{17.4}$$

It is then observed in [HR87] that, using the formal rule (17.3), the Gaussian integral evaluates as

$$\begin{aligned}\int_{-\infty}^{\infty} e^{-\alpha x^2}\,\mathrm{d}^D x &= \sum_n \frac{(-\alpha)^n}{n!}\int_{-\infty}^{\infty}(x^2)^n \mathrm{d}^D x \\ &= \sum_n \frac{(-\alpha)^n}{n!}(-1)^n \pi^{D/2}\Gamma(n+1)\;\delta_{n+D/2,0} \\ &= \left(\frac{\pi}{\alpha}\right)^{D/2}.\end{aligned} \tag{17.5}$$

In turn, the formal equality

$$\sum_n \frac{(-\alpha)^n}{n!} \int_{-\infty}^{\infty} (x^2)^n \mathrm{d}^D x = \left(\frac{\pi}{\alpha}\right)^{D/2}$$

may be used to motivate the definition (17.3).

The method of brackets, as first presented in [GS07], started from the same underlying idea. Instead of formally expanding the Gaussian integral (17.5), one expands

$$\frac{\Gamma(s)}{\alpha^s} = \int_0^{\infty} x^{s-1} e^{-\alpha x}\,\mathrm{d}x = \sum_n \frac{(-\alpha)^n}{n!} \int_0^{\infty} x^{n+s-1}\,\mathrm{d}x,$$

which leads to the formal definition [GS07, (A.2)]

$$\int_0^{\infty} x^{n+s-1}\,\mathrm{d}x = \frac{\Gamma(s)\Gamma(n+1)}{(-1)^n}\delta_{n+s,0}. \tag{17.6}$$

Gonzalez and Schmidt then introduce the notation $\langle n+s\rangle$ for the left-hand side and go on to develop the formal rules that are presented in Section 8.9 of Chapter 8.

One advantage of the modified approach (17.6) over the original (17.3) is that it is easier to apply to integrals outside the context of Feynman integrals. A variety of examples is given in [GM10].

17.1.2 Mellin–Barnes integrals

Another standard practice, especially in particle physics [Smi06], is the introduction of Mellin–Barnes representations to evaluate definite integrals. The final (multiple) Mellin–Barnes integral may then be solved by closing the contours and collecting the appropriate residues. By way of several examples, we will illustrate that an application of the method of brackets corresponds to a way of systematically introducing Mellin–Barnes representations. The rigor that may be obtained in this fashion comes at the price of introducing, along the way, arguably more technically involved contour integrals and having to collect appropriate sets of residues.

We begin by illustrating the correspondence by observing that a Taylor expansion of a function $f(x)$ may be expressed as a Mellin–Barnes integral representation. Namely, if

$$f(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} a(n) x^n, \tag{17.7}$$

then, by Ramanujan's Master Theorem and under appropriate conditions on $a(n)$ as stated for instance in Theorem 8.3.2, we have

$$\int_0^\infty x^{s-1} f(x)\,\mathrm{d}x = \Gamma(s) a(-s). \tag{17.8}$$

Hence, by Mellin inversion, proved in Theorem 17.1.6, $f(x)$ has the Mellin–Barnes integral representation

$$f(x) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \Gamma(s) a(-s) x^{-s}\,\mathrm{d}s. \tag{17.9}$$

Here, and below, the exact contour is meant to be chosen appropriately. In this case that means that the poles of $\Gamma(s)$ lie to the left of the contour and that, on this side, $a(-s)$ is analytic.

Example 17.1.1. In the case $f(x) = \frac{1}{1+x}$ we have $a(n) = \Gamma(n+1)$ and hence

$$\frac{1}{1+x} = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \Gamma(s)\Gamma(1-s) x^{-s}\,\mathrm{d}s. \tag{17.10}$$

We remark that closing the contour to the left reproduces the Taylor expansion of $f(x)$ at 0 which converges for $|x| < 1$. The Mellin–Barnes representation of $f(x)$ also allows the contour to be closed to the right. In that case, one sums the residues at the poles $s = n+1$ for $n = 0, 1, \dots$ to obtain the series

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \Gamma(n+1) x^{-(n+1)} = \frac{1}{x} \frac{1}{1+\frac{1}{x}} = \frac{1}{1+x},$$

which also represents $f(x)$, but now for $|x| > 1$. It is this well-known aspect of Mellin–Barnes representations [AAR99] that is responsible for the fact that the method of brackets is able to give different evaluations of a given integral which are valid in different regions and analytic continuations of each other.

The bracket expansion

$$\frac{1}{(a_1+a_2)^{\alpha}} = \sum_{m_1, m_2} \frac{(-1)^{m_1+m_2}}{m_1! m_2!} a_1^{m_1} a_2^{m_2} \frac{\langle \alpha + m_1 + m_2 \rangle}{\Gamma(\alpha)} \tag{17.11}$$

stated more generally as Rule 8.9.1 has the following Mellin–Barnes analog:

$$\frac{1}{(a_1+a_2)^{\alpha}} = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \frac{\Gamma(-s)\Gamma(\alpha+s)}{\Gamma(\alpha)} a_1^s a_2^{-\alpha-s} \, \mathrm{d}s \tag{17.12}$$

Here, $|\arg a_1 - \arg a_2| < \pi$ and the contour is understood to be such that it separates the poles $s = 0, 1, 2, \dots$ of $\Gamma(-s)$ from the poles $s = -\alpha, -\alpha-1, \dots$ of $\Gamma(\alpha+s)$.

Remark 17.1.2. Equation (17.12) is a special case of the Mellin–Barnes representation, see [PK01, Section 3.4.2], for the hypergeometric function, valid for $|\arg(x)| < \pi$,

$$\frac{\Gamma(a)\Gamma(b)}{\Gamma(c)} {}_2F_1\left(\left. \begin{matrix} a, b \\ c \end{matrix} \right| -x \right) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \frac{\Gamma(a+s)\Gamma(b+s)}{\Gamma(c+s)} \Gamma(-s) x^s \, \mathrm{d}s,$$

and the fact that, when $b = c$, the left-hand side reduces to $\frac{\Gamma(a)}{(1+x)^a}$.

In a sequence of examples we now show how these tools, coupled with the inverse Mellin transform which is shortly reviewed in Section 17.1.3, allow evaluation of definite integrals along the lines of an application of the method of brackets.

Example 17.1.3. As in Section 8.9.1 we consider, for illustration, the integral

$$\int_0^\infty \int_0^\infty x^{s-1} y^{t-1} \exp\left(-(x+y)^\alpha\right) \, \mathrm{d}x \, \mathrm{d}y.$$

Using the Mellin–Barnes integral (17.9) for the exponential function, followed by an application of (17.12), we have

$$\begin{aligned}
\exp\left(-(x+y)^\alpha\right) &= \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \Gamma(\sigma)(x+y)^{-\sigma\alpha} \, \mathrm{d}\sigma \\
&= \frac{1}{(2\pi i)^2} \int_{-i\infty}^{i\infty} \int_{-i\infty}^{i\infty} \frac{\Gamma(\sigma)\Gamma(-\tau)\Gamma(\sigma\alpha+\tau)}{\Gamma(\sigma\alpha)} x^\tau y^{-\sigma\alpha-\tau} \, \mathrm{d}\tau \, \mathrm{d}\sigma \\
&= \frac{1}{(2\pi i)^2} \int_{-i\infty}^{i\infty} \int_{-i\infty}^{i\infty} \frac{1}{\alpha} \frac{\Gamma(\frac{s+t}{\alpha})\Gamma(s)\Gamma(t)}{\Gamma(s+t)} x^{-s} y^{-t} \, \mathrm{d}s \, \mathrm{d}t.
\end{aligned}$$

In the last step we performed the change of variables $-s = \tau$ and $-t = -\sigma\alpha - \tau$. Thus an application of the (multiple) inverse Mellin transform, stated as Theorem 17.1.6, yields the integral evaluation

$$\int_0^\infty \int_0^\infty x^{s-1} y^{t-1} \exp\left(-(x+y)^\alpha\right) \, \mathrm{d}x \, \mathrm{d}y = \frac{1}{\alpha} \frac{\Gamma(\frac{s+t}{\alpha})\Gamma(s)\Gamma(t)}{\Gamma(s+t)}.$$

This agrees with the result obtained in Section 8.9.1 using the method of brackets.

Example 17.1.4. Consider, for $\alpha, \beta, \nu > 0$, the integral

$$\int_0^\infty x^\nu e^{-\alpha x} J_\nu(\beta x) \, \mathrm{d}x = \frac{(2\beta)^\nu \Gamma(\nu + \frac{1}{2})}{\sqrt{\pi}(\alpha^2 + \beta^2)^{\nu+1/2}} \tag{17.13}$$

that was evaluated in Section 9.3 using the method of brackets. The relevant Mellin–Barnes representations, equivalent through (17.9) to the respective Taylor expansions, are

$$e^{-\alpha x} = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{\Gamma(s)}{\alpha^s} x^{-s}\,\mathrm{d}s,$$
$$x^{\nu} J_{\nu}(\beta x) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{1}{2}\left(\frac{2}{\beta}\right)^{t+\nu} \frac{\Gamma(\nu+\frac{t}{2})}{\Gamma(1-\frac{t}{2})} x^{-t}\,\mathrm{d}t,$$

valid for $\operatorname{Re} s > 0$ and $-2\nu < \operatorname{Re} t < 3/2 - \nu$, respectively. Recall that the contour integrals are understood to seperate the increasing from the decreasing sequence of poles.

After the change of variables $u = s + t$, $v = t/2$, we have

$$e^{-\alpha x} x^{\nu} J_{\nu}(\beta x) = \frac{1}{(2\pi i)^2}\int_{-i\infty}^{i\infty}\int_{-i\infty}^{i\infty} \frac{\Gamma(u-2v)}{\alpha^{u-2v}}\left(\frac{2}{\beta}\right)^{2v+\nu} \frac{\Gamma(\nu+v)}{\Gamma(1-v)} x^{-u}\,\mathrm{d}v\,\mathrm{d}u.$$

It then follows that the left-hand side of (17.13) is given by setting $u = 1$ in

$$\int_0^{\infty} x^{u+\nu-1} e^{-\alpha x} J_{\nu}(\beta x)\,\mathrm{d}x = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{\Gamma(u-2v)}{\alpha^{u-2v}}\left(\frac{2}{\beta}\right)^{2v+\nu} \frac{\Gamma(\nu+v)}{\Gamma(1-v)}\,\mathrm{d}v. \tag{17.14}$$

Note that the integrand has two sequences of poles: an increasing sequence of poles at $2v = u, u+1, u+2, \dots$ and a decreasing sequence of poles at $v = -\nu, -\nu-1, -\nu-2, \dots$. Closing the contour to the left, that is collecting the residues of the poles at $v = -\nu-n$ for $n \in \mathbb{Z}_{\geqslant 0}$, yields

$$\frac{1}{\alpha^{u+\nu}}\sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\frac{\Gamma(u+2\nu+2n)}{\Gamma(1+\nu+n)}\left(\frac{\beta}{2\alpha}\right)^{\nu+2n}.$$

In the case $u = 1$ this is precisely the series (9.12) obtained previously by the method of brackets. In particular, one obtains, for $|\beta| < |\alpha|$, the evaluation (17.13).

On the other hand, closing the contour in (17.14) to the right, yields the series

$$\frac{1}{2}\left(\frac{2}{\beta}\right)^{u+\nu}\sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\left(\frac{2\alpha}{\beta}\right)^{n} \frac{\Gamma(\nu+u/2+n/2)}{\Gamma(1-u/2-n/2)},$$

which, for $u=1$, coincides with (9.14). This second series converges for $|\beta| > |\alpha|$.

Example 17.1.5. In this example we will illustrate the heuristic Rule 8.9.3 of the method of brackets by evaluating the integral

$$\int_0^\infty J_0(\alpha x)\frac{x^{s-1}}{(1+x^2)^\lambda}\,\mathrm{d}x, \tag{17.15}$$

first by employing the method of brackets and then, in the corresponding fashion, by the Mellin–Barnes approach. For this integral, the method of brackets yields three bracket series, one of which is divergent. The two other series converge in a common region and add up to (17.15). This is confirmed in the Mellin–Barnes approach which results in a Mellin–Barnes contour integral representing (17.15): closing the contour to the right produces a divergent asymptotic expansion while closing the contour to the left results in two series of residues which together give (17.15).

Applying the method of brackets, we have

$$\begin{aligned}
&\int_0^\infty J_0(\alpha x)\frac{x^{s-1}}{(1+x^2)^\lambda}\,\mathrm{d}x \\
&\qquad = \sum_k \phi_k \int_0^\infty \left(\frac{\alpha}{2}\right)^{2k}\frac{1}{\Gamma(k+1)}\frac{x^{2k+s-1}}{(1+x^2)^\lambda}\,\mathrm{d}x \\
&\qquad = \frac{1}{\Gamma(\lambda)}\sum_{k,n,m}\phi_{k,n,m}\left(\frac{\alpha}{2}\right)^{2k}\frac{1}{\Gamma(k+1)}\langle n+m+\lambda\rangle\,\langle 2m+2k+s\rangle\,.
\end{aligned}$$

There are 3 indices and 2 brackets which leaves 1 free variable to be chosen. If k is chosen as the free variable, then $m^* = -k-\frac{s}{2}$ and $n^* = -\lambda+k+\frac{s}{2}$. Since $|\det| = 2$, the contribution is

$$\begin{aligned}
&\frac{1}{2\Gamma(\lambda)}\sum_k \phi_k \left(\frac{\alpha}{2}\right)^{2k} \frac{1}{\Gamma(k+1)}\Gamma(-n^*)\Gamma(-m^*) \\
&= \frac{1}{2\Gamma(\lambda)}\sum_k \frac{(-1)^k}{(k!)^2}\left(\frac{\alpha}{2}\right)^{2k}\Gamma(\lambda-k-\tfrac{s}{2})\Gamma(k+\tfrac{s}{2}) \\
&= \frac{\Gamma(\frac{s}{2})\Gamma(\lambda-\frac{s}{2})}{2\Gamma(\lambda)}\,{}_1F_2\left(\left.\begin{matrix}\frac{s}{2}\\ 1, 1-\lambda+\frac{s}{2}\end{matrix}\right|\frac{\alpha^2}{4}\right).
\end{aligned} \tag{17.16}$$

This converges for $\left|\frac{\alpha^2}{4}\right| < 1$. Similarly, the contribution with n as the free variable is

$$\left(\frac{\alpha}{2}\right)^{2\lambda-s}\frac{\Gamma(-\lambda+\frac{s}{2})}{2\Gamma(\lambda+1-\frac{s}{2})}\,{}_1F_2\left(\left.\begin{matrix}\lambda\\ 1+\lambda-\frac{s}{2}, 1+\lambda-\frac{s}{2}\end{matrix}\right|\frac{\alpha^2}{4}\right), \tag{17.17}$$

which converges in the same region. On the other hand, with m as free variable one obtains the divergent series

$$\frac{1}{2\Gamma(\lambda)}\sum_m \frac{(-1)^m}{m!}\left(\frac{\alpha}{2}\right)^{-2m-s}\frac{\Gamma(m+\lambda)\Gamma(m+\frac{s}{2})}{\Gamma(1-m-\frac{s}{2})}. \tag{17.18}$$

Combining the two convergent series, we therefore have the evaluation

$$\begin{aligned}
\int_0^\infty J_0(\alpha x)\frac{x^{s-1}}{(1+x^2)^\lambda}\,\mathrm{d}x &= \frac{\Gamma(\frac{s}{2})\Gamma(\lambda-\frac{s}{2})}{2\Gamma(\lambda)}\,{}_1F_2\left(\left.\begin{matrix}\frac{s}{2}\\ 1, 1-\lambda+\frac{s}{2}\end{matrix}\right|\frac{\alpha^2}{4}\right) \\
&+ \left(\frac{\alpha}{2}\right)^{2\lambda-s}\frac{\Gamma(-\lambda+\frac{s}{2})}{2\Gamma(\lambda+1-\frac{s}{2})}\,{}_1F_2\left(\left.\begin{matrix}\lambda\\ 1+\lambda-\frac{s}{2}, 1+\lambda-\frac{s}{2}\end{matrix}\right|\frac{\alpha^2}{4}\right).
\end{aligned}$$

We remark that in the special case $s = 2$ this combines pleasantly to

$$\int_0^\infty J_0(\alpha x)\frac{x}{(1+x^2)^{\lambda+1}}\,\mathrm{d}x = \left(\frac{\alpha}{2}\right)^\lambda \frac{K_\lambda(\alpha)}{\lambda!},$$

and, even more specially,

$$\int_0^\infty J_0(\alpha x)\frac{x}{(1+x^2)^{3/2}}\,\mathrm{d}x = \mathrm{e}^{-\alpha}.$$

Let us now evaluate (17.15) by using the Mellin–Barnes approach. In that case we commence with

$$J_0(\alpha x) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{1}{2}\left(\frac{2}{\alpha}\right)^s \frac{\Gamma(s/2)}{\Gamma(1-s/2)} x^{-s}\,\mathrm{d}s$$

which, as in (17.9), is equivalent to the series expansion of $J_0(\alpha x)$. By (17.12), introduced as the analog of Rule 8.9.1, we further have

$$\frac{1}{(1+x^2)^\lambda} = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{\Gamma(-t)\Gamma(\lambda+t)}{\Gamma(\lambda)} x^{2t}\,\mathrm{d}t.$$

Hence, after the change of variables $u = s - 2t$,

$$\frac{J_0(\alpha x)}{(1+x^2)^\lambda} = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \left[\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{1}{2}\left(\frac{2}{\alpha}\right)^{u+2t} \frac{\Gamma(u/2+t)\Gamma(-t)\Gamma(\lambda+t)}{\Gamma(1-u/2-t)\Gamma(\lambda)}\,\mathrm{d}t\right] x^{-u}\,\mathrm{d}u.$$

By the Mellin inversion formula, Theorem 17.1.6, it follows that

$$\int_0^\infty J_0(\alpha x)\frac{x^{s-1}}{(1+x^2)^\lambda}\,\mathrm{d}x = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \frac{1}{2}\left(\frac{2}{\alpha}\right)^{s+2t} \frac{\Gamma(s/2+t)\Gamma(-t)\Gamma(\lambda+t)}{\Gamma(1-s/2-t)\Gamma(\lambda)}\,\mathrm{d}t. \tag{17.19}$$

The integrand has decreasing sequences of poles at $t = -s/2 - n$ and $t = -\lambda - n$ for $n \in \mathbb{Z}_{\geqslant 0}$. The residues of the poles at $t = -s/2 - n$ sum to

$$\frac{1}{2}\sum_{n=0}^\infty \frac{(-1)^n}{n!}\left(\frac{\alpha}{2}\right)^{2n} \frac{\Gamma(s/2+n)\Gamma(\lambda-s/2-n)}{\Gamma(1+n)\Gamma(\lambda)}, \tag{17.20}$$

which coincides with (17.16). Likewise the residues of the poles at $t = -\lambda - n$ sum to

$$\frac{1}{2}\sum_{n=0}^\infty \frac{(-1)^n}{n!}\left(\frac{\alpha}{2}\right)^{2n+2\lambda-s} \frac{\Gamma(\lambda+n)\Gamma(s/2-\lambda-n)}{\Gamma(1-s/2+\lambda+n)\Gamma(\lambda)}, \tag{17.21}$$

which rewrites to (17.17). If, on the other hand, one closes the contour in (17.19) to the right then the residues at $t = 0, 1, 2, \ldots$ yield the divergent asymptotic expansion

(17.18).

17.1.3 Mellin transform

For completeness and convenience of the reader we include here a proof of the Mellin inversion theorem which is at the heart of Section 17.1.2. The proof given here is adopted from the two-dimensional case discussed in [Ree44, Fox57] which is based on Mellin's original treatment; it thus is most likely precisely the classical one.

Theorem 17.1.6 (Mellin inversion formula)**.** *Assume that $F(s)$ is analytic in the strip $a < \mathrm{Re}\ s < b$ and that $F(s) \to 0$ as $|\mathrm{Im}\ s| \to \infty$. upon restricting to compact [a',b']) Define f by*

$$f(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} F(s) x^{-s}\, \mathrm{d}s. \tag{17.22}$$

If this integral converges absolutely for all $c \in (a, b)$, then

$$F(s) = \int_0^\infty x^{s-1} f(x)\, \mathrm{d}x.$$

Proof. First, note that the integral (17.22) does not depend on the specific value of $c \in (a, b)$. Given s with $a < \mathrm{Re}\ s < b$ we can therefore write, for any c_1, c_2 satisfying $a < c_1 < \mathrm{Re}\ s < c_2 < b$,

$$\begin{aligned}\int_0^\infty x^{s-1} f(x)\, \mathrm{d}x &= \int_0^1 x^{s-1} \frac{1}{2\pi i} \int_{c_1-i\infty}^{c_1+i\infty} F(t) x^{-t}\, \mathrm{d}t\, \mathrm{d}x \\ &\quad + \int_1^\infty x^{s-1} \frac{1}{2\pi i} \int_{c_2-i\infty}^{c_2+i\infty} F(t) x^{-t}\, \mathrm{d}t\, \mathrm{d}x \\ &= -\frac{1}{2\pi i} \int_{c_1-i\infty}^{c_1+i\infty} \frac{F(t)}{t-s}\, \mathrm{d}t + \frac{1}{2\pi i} \int_{c_2-i\infty}^{c_2+i\infty} \frac{F(t)}{t-s}\, \mathrm{d}t,\end{aligned}$$

where in the last step we used that the involved integrals are absolutely convergent to justify switching the order of integration. By Cauchy's residue theorem we have, for $M > |\,\mathrm{Im}\ s|$,

$$\frac{1}{2\pi i}\left[\int_{c_2-iM}^{c_2+iM} - \int_{c_1+iM}^{c_2+iM} - \int_{c_1-iM}^{c_1+iM} + \int_{c_1-iM}^{c_2-iM}\right]\frac{F(t)}{t-s}\,\mathrm{d}t = F(s).$$

By the assumed convergence $F(t) \to 0$ as $|\,\mathrm{Im}\ t| \to \infty$, the two auxiliary horizontal line integrals vanish as $M \to \infty$. Hence

$$\int_0^\infty x^{s-1} f(x)\,\mathrm{d}x = F(s)$$

as claimed. □

The Mellin inversion theorem and its proof extend to several variables. The two-dimensional case, which results in no loss of generality, is proven in [Ree44] along the lines of the proof just given.

Theorem 17.1.7. *Assume that $F(s_1, \ldots, s_n)$, as a function of s_k, is analytic in the strip $a_k < \mathrm{Re}\ s_k < b_k$ for each $k = 1, \ldots, n$. Further, assume that $F(s_1, \ldots, s_n) \to 0$ as $|\,\mathrm{Im}\ s_1|, \ldots, |\,\mathrm{Im}\ s_n| \to \infty$, independently of each other. Define f by*

$$f(x_1, \ldots, x_n) = \frac{1}{(2\pi i)^n}\int_{c_1-i\infty}^{c_1+i\infty} \cdots \int_{c_n-i\infty}^{c_n+i\infty} F(s_1, \ldots, s_n) x_1^{-s_1} \cdots x_n^{-s_n}\,\mathrm{d}s_1 \cdots \mathrm{d}s_n. \tag{17.23}$$

If this integral converges absolutely for all $c_1, \ldots, c_n$ with $c_k \in (a_k, b_k)$ then

$$F(s_1, \ldots, s_n) = \int_0^\infty \cdots \int_0^\infty x_1^{s_1-1} \cdots x_n^{s_n-1} f(x_1, \ldots, x_n)\,\mathrm{d}x_1 \cdots \mathrm{d}x_n.$$

17.2 Creative telescoping leading to divergent integrals

In this section, we apply the creative telescoping approach to the problem, considered in Chapter 4, of obtaining the differential equation satisfied by the probability density function p_4. This problem splits into two parts: *finding* the differential equation and *proving* that p_4 is one of its solutions. As we are going to illustrate, the first part of this problem is straightforward to solve using creative telescoping. Yet, the step of proving, which in other applications of creative telescoping often reduces to routine verification, poses certain issues, described below, which include that applying differential operators and taking limits do not commute. We do not offer a satisfactory resolution but remark that a general approach to solving the issues at hand would be interesting: when deducing the differential equation in Chapter 4 we had to use the *distributional* Mellin transform to work around the issues.

The probability density of the distance travelled by a four-step random walk, as discussed in Chapter 4, is

$$p_4(x) = \int_0^\infty xtJ_0(t)^4 J_0(xt)\,\mathrm{d}t, \tag{17.24}$$

where J_0 is a Bessel function. Using Mellin calculus and the relation of p_4 to the moments W_4, it was shown in Example 4.2.3 of Chapter 4 that p_4 satisfies the differential equation $A_4 \cdot p_4 = 0$ with

$$\begin{aligned} A_4 &= x^4(\theta+1)^3 - 4x^2\theta(5\theta^2+3) + 64(\theta-1)^3 \\ &= (x-4)(x-2)x^3(x+2)(x+4)D_x^3 + 6x^4\left(x^2-10\right)D_x^2 \\ &\quad + x\left(7x^4-32x^2+64\right)D_x + \left(x^2-8\right)\left(x^2+8\right). \end{aligned} \tag{17.25}$$

Here $\theta = xD_x = x\frac{\mathrm{d}}{\mathrm{d}x}$.

In this section, we will discuss the issue of finding and establishing this differential equation using creative telescoping. A nice introduction to the ideas underlying creative telescoping is [PWZ96], and a very useful implementation (in *Mathematica*) of the creative telescoping algorithm is given in the package `HolonomicFunctions` [Kou10] by Christoph Koutschan.

We denote the integrand of (17.24) by $f_4(x,t) = xtJ_0(t)^4 J_0(xt)$. Using creative telescoping we find operators $A = A(x, D_x)$ and $B = B(x, D_x, t, D_t)$ such that

$$(A + D_t B) \cdot f_4 = 0. \tag{17.26}$$

Indeed, using for instance `HolonomicFunctions`, we obtain

$$\begin{aligned}
A &= A_4,\\
B &= t^3x^2D_t^4 + 7t^2x^2D_t^3 - 5t^2x^3D_xD_t^3 - tx^2\left(10x^2t^2 - 20t^2 - 1\right)D_t^2\\
&\quad - 4x^2\left(5x^2t^2 - 15t^2 - 1\right)D_t + 5x^3\left(2x^2t^2 - 12t^2 - 1\right)D_xD_t\\
&\quad + \frac{x^2\left(5x^4t^4 - 60x^2t^4 + 64t^4 - 28t^2 - 4\right)}{t} - \frac{5x^3\left(2x^2t^2 - 12t^2 - 1\right)D_x}{t}.
\end{aligned}$$

Note that the operator A found by creative telescoping coincides with the differential operator A_4 from (17.25). In other words, we succeeded in *finding* the differential equation we were looking for.

The second step is to use the relation (17.26) to *show* that p_4 indeed solves the differential equation $A \cdot p_4 = 0$. However,

$$A \cdot \int_0^t f_4(x,s)\mathrm{d}s = \int_0^t A \cdot f_4(x,s)\mathrm{d}s = \int_0^t -D_tB \cdot f_4(x,s)\mathrm{d}s = -B \cdot f_4(x,t) \tag{17.27}$$

and the right-hand side does not converge as $t \to \infty$. This is illustrated for $x = 3/2$ in Figure 17.1.

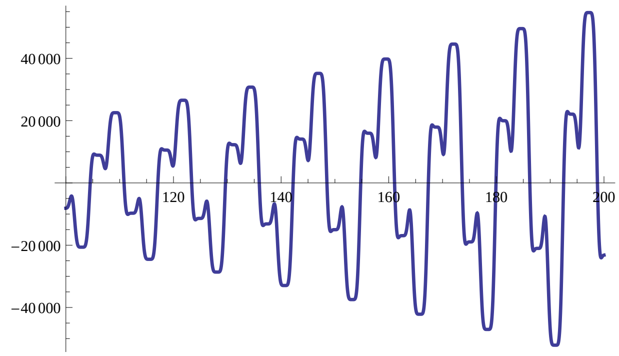


Figure 17.1: $-B \cdot f_4(3/2, t)$

In fact, it is not true that, as $t \to \infty$,

$$D_x^n \cdot \int_0^t f_4(x,s)\mathrm{d}s \longrightarrow D_x^n \cdot \int_0^\infty f_4(x,s)\mathrm{d}s = p_4^{(n)}(x). \tag{17.28}$$

To see the failure of (17.28), note that in the case $n = 2$

$$D_x^2 \cdot \int_0^t f_4(x,s)\mathrm{d}s = \int_0^t D_x^2 \cdot f_4(x,s)\mathrm{d}s = -\int_0^t s^2 J_0(s)^4 \left(xsJ_0(xs) + J_1(xs)\right) \mathrm{d}s. \tag{17.29}$$

In light of the asymptotic form

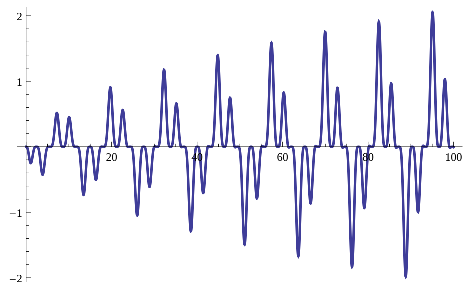
$$J_\alpha(x) \approx \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\alpha\pi}{2} - \frac{\pi}{4}\right),$$

the integral (17.29) is seen to not converge as $t \to \infty$. The integrand and the integral are depicted in Figure 17.2.

It is unclear to the author how to proceed from here.

Remark 17.2.1. From (17.27), as suggested by Manuel Kauers, one can proceed by seeking an operator $C = C(x, D_x, t)$ which annihilates the right-hand side of (17.27). For such C and for all $t > 0$, we will then have

$$CA \cdot \int_0^t f_4(x,s)\mathrm{d}s = 0. \tag{17.30}$$



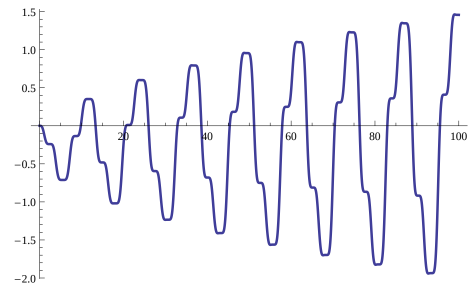


Figure 17.2: The integrand of the RHS of (17.29) and the integral (17.29) when $x = 1/2$

Using, for instance, once more the functionality of the package `HolonomicFunctions` we indeed find such C of order 10 in D_x and degree 10 in both x and t. Moreover, the only monomial in C which involves t^{10} is of the form $x^{10}t^{10}$; in other words,

$$\frac{C}{t^{10}} \longrightarrow x^{10} \quad \text{as } t \to \infty.$$

At this point, we would like to take the limit $t \to \infty$ in (17.30) after dividing both sides by t^{10}. If possible, this would allow us to conclude that $x^{10}A \cdot p_4 = 0$ which, of course, implies $A \cdot p_4 = 0$. In light of (17.28), there is, however, similar trouble as in (17.27): the limit $t \to \infty$ in (17.30) can not be taken individually for each monomial of CA.

Remark 17.2.2. Maybe it is worth pointing out that the integral (17.29) as $t \to \infty$ seems to approach the desired value $p_4''(x)$ in a certain "average sense": as illustrated in Figure 17.3, the oscillations, though increasing in magnitude, appear to stabilize about $p_4''(x)$. The same phenomenon can be observed in equation (17.27) and Figure 17.1 where the desired value is zero.

Remark 17.2.3. As suggested by Doron Zeilberger, one way to circumvent the appearance of integrals that do not converge is to replace the integrand $f_4(x, t)$ by $e^{-\lambda t} f_4(x, t)$ with an extra parameter $\lambda > 0$. In other words, instead of for p_4, as in

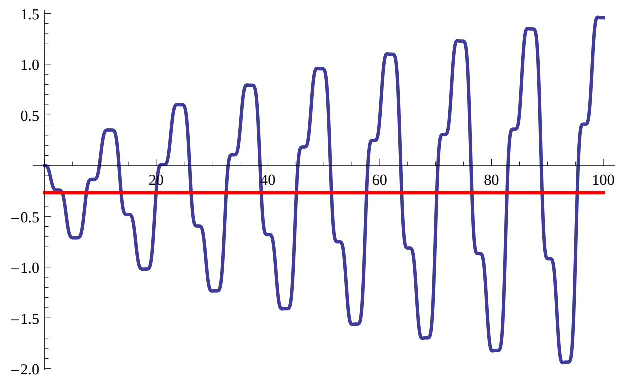


Figure 17.3: The integral (17.29) when $x = 1/2$ with $p_4''(1/2) = -0.266$ superimposed

(17.24), we set out to find a differential equation for

$$\int_0^\infty xtJ_0(t)^4 J_0(xt)e^{-\lambda t}\,\mathrm{d}t. \tag{17.31}$$

In the resulting equations we finally take the limit $\lambda \to 0$.

While this approach can solve the problem of finding and proving a differential equation for p_4, it does so not via the relation (17.26) for the integrand $f_4(x,t)$ but via a corresponding relation for the generalized integrand $e^{-\lambda t} f_4(x,t)$. This latter relation, as well as finding it, is much more involved. It would be nice to deduce, by some general principle, the differential equation directly from (17.26).

In conclusion, it would be very interesting to have an a priori reason of some sort that would allow us to conclude (in this and other cases) that the differential operator $A + D_t B$, from (17.26), found by the creative telescoping method yields the desired differential operator A annihilating p_4 (even though we cannot do the usual interchange of differentiation and integration). In light of Remark 17.2.2 and the success of the distributional Mellin transform in this instance, distributions may well be the right framework for further insight.

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Biography

Armin Straub graduated with a diploma in Mathematics and a minor in Computer Science from Technische Universität Darmstadt, Germany, in 2008 under the guidance of Ralf Köhl. During his time at Darmstadt he had spent the academic year of 2006/2007 at Tulane University as part of an exchange program initiated by Karl H. Hofmann. At Tulane University he obtained a master's degree and started to learn from and work with Victor H. Moll and Tewodros Amdeberhan. Completing his diploma at Darmstadt, Armin therefore returned to New Orleans in 2008 to pursue a doctoral degree under the guidance of Victor Moll. In the summer of 2009, he had the chance to visit Jonathan M. Borwein at Newcastle University, Australia, which has resulted in ongoing collaboration and two further visits including a semester-long stay at Newcastle University in Fall 2010.

Beginning Fall 2012, Armin will be J. L. Doob Research Assistant Professor at the University of Illinois at Urbana-Champaign, working with Bruce Berndt. During the academic year 2013 he will take a leave to visit the Max-Planck Institute in Bonn, Germany. Armin is very excited about both.