

Random Walks, Elliptic Integrals and Related Constants

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Statement of Originality

The thesis contains no material which has been accepted for the award of any other degree or diploma in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text. I give consent to the final version of my thesis being made available worldwide when deposited in the University's Digital Repository, subject to the provisions of the Copyright Act 1968.

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Extent of Collaboration and Authorship

A number of chapters in this dissertation have appeared in or been accepted for publication. All of them have been significantly edited (solely by me) from their published versions. In particular, each chapter contains new material. Since joint scholarly projects result from the synergy of individual contributions, it is impractical to break down such projects into the works of each coauthor. I have been a significant and integral contributor in all my joint papers, and below I will only highlight the parts for which I was close to being the sole contributor.

Chapters 4, 7, 8, 12 and 14 are solely my work. They have not appeared in print, except: Section 7.9 is a paraphrasing of my unpublished joint article [169], Section 8.4 comes from my contribution to the published joint paper [41], Section 12.5 has been placed on-line [191], and a brief summary of Section 14.3 will appear in the book [52].

Chapter 6 is based on my published paper [190]; the first 4 sections of **Chapter 13** are based on my accepted paper [192] (the next 2 sections are my work that have not appeared in print).

The bulk of **Chapter 1** is based on the published joint paper [53]; I was responsible for much of the crucial development in Section 1.2, which initiated the research. **Chapter 2** is mostly based on the published joint paper [56]; I obtained and proved some of the theorems in Sections 2.2 and 2.3. **Chapter 3** is largely adapted from the published joint paper [57]; I contributed much to Section 3.4, and Sections 3.6 and 3.7 were mostly my work. **Chapter 5** is edited from the published joint paper [40]; I was responsible for a number of results, for instance theorem 5.6. **Chapter 9** is a significantly altered version of the published joint paper [41]; I was responsible for some of the analysis in Sections 9.5 and 9.6, and new material has been inserted. Most of **Chapter 10** comes from the published joint paper [74]. I was responsible for all the computations, and for Section 10.8; some materials in Sections 10.3 and 10.5 have not appeared in print; Section 10.10 is based on the published joint paper [73], where I contributed to the last part. **Chapter 11** follows closely the published

joint paper [193]; I performed all the computations and discovered the main result (theorem 11.1), while the proof of the theorem was an extensive collaborative effort between the two authors.

Declaration by the candidate

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Endorsement by the supervisor

I, as the supervisor of the candidate, certify that the details provided above are correct.

Supervisor name: _____

Supervisor signature: _____ Date: _____

Contents

Chapter 0. Introduction	xi
0.1. Acknowledgments	xii
0.2. Overview	xvi
Chapter 1. Arithmetic Properties of Short Random Walk Integrals	1
1.1. Introduction, history and preliminaries	1
1.2. The even moments and their combinatorial features	5
1.3. Analytic features of the moments	11
1.4. Bessel integral representations	15
1.5. The odd moments of a three-step walk	15
1.6. Appendix: Numerical evaluations	19
Chapter 2. Three-Step and Four-Step Random Walk Integrals	21
2.1. Introduction and preliminaries	21
2.2. Bessel integral representations	22
2.3. Probabilistically inspired representations	33
2.4. Partial resolution of the conjecture	39
Chapter 3. Densities of Short Uniform Random Walks	41
3.1. Introduction	41
3.2. The densities p_n	43
3.3. The density p_3	46
3.4. The density p_4	47
3.5. The density p_5	54
3.6. Derivative evaluations of W_n	56
3.7. New results on W_n	61
Chapter 4. More Results on Uniform Random Walks	67
4.1. Elementary derivations of p_2 and p_3	67

4.2.	Three-step walk with different step lengths	69
4.3.	Higher dimensions	71
4.4.	Limiting the number of directions	77
Chapter 5. Moments of Elliptic Integrals and Catalan's Constant		79
5.1.	Introduction and background	79
5.2.	Basic results	82
5.3.	Closed form initial values	88
5.4.	Contour integrals for G_s	91
5.5.	Closed forms at negative integers	92
Chapter 6. Moments of Products of Elliptic Integrals		95
6.1.	Motivation and general approach	95
6.2.	One elliptic integral	97
6.3.	Two complementary elliptic integrals	98
6.4.	One elliptic integral and one complementary elliptic integral	102
6.5.	Sporadic results	105
6.6.	Fourier series	107
6.7.	Legendre's relation	109
6.8.	Integration by parts	110
Chapter 7. More Integrals of K and E		119
7.1.	One elliptic and one complementary elliptic integral	119
7.2.	Two complementary elliptic integrals	122
7.3.	Two elliptic integrals	123
7.4.	More on explicit primitives	125
7.5.	Some other integrals	126
7.6.	Incomplete moments	129
7.7.	One elliptic integral with parameters	130
7.8.	Fourier series and three elliptic integrals	132
7.9.	Proof of the conjecture	134
7.10.	Some hypergeometric identities	138
Chapter 8. Elementary Evaluations of Mahler Measures		141
8.1.	Jensen's formula and Mahler measures	141

8.2.	On $\mu(k + x + 1/x + y + 1/y)$	148
8.3.	On $\mu((1 + x)(1 + y) + z)$.	150
8.4.	Proofs of two conjectures of Boyd	151
Chapter 9. Log-sine Evaluations of Mahler Measures		155
9.1.	Introduction	155
9.2.	Preliminaries and log-sine integrals	156
9.3.	Mahler measures and moments of random walks	160
9.4.	Epsilon expansion of W_3	161
9.5.	Trigonometric analysis of $\mu_n(1 + x + y)$	164
9.6.	Evaluation of $\mu_2(1 + x + y)$	172
Chapter 10. Legendre Polynomials and Ramanujan-type Series for $1/\pi$		175
10.1.	Introduction	175
10.2.	Brafman's formula and modular equations	176
10.3.	Identities for $s = 1/2$	181
10.4.	Identities for $s = 1/3$	184
10.5.	Identities for $s = 1/4$	187
10.6.	New identities for $s = 1/6$	191
10.7.	Companion series	192
10.8.	Closed forms	193
10.9.	Summary	194
10.10.	Complex Series for $1/\pi$	195
Chapter 11. Generating Functions of Legendre Polynomials		203
11.1.	Introduction	203
11.2.	Apéry-like sequences	206
11.3.	Generalised Bailey's identity	209
11.4.	Generating functions of Legendre polynomials	210
11.5.	Formulas for $1/\pi$	212
11.6.	Concluding remarks	218
Chapter 12. New Series for $1/\pi$		221
12.1.	Orthogonal polynomials	221
12.2.	Orr-type theorems and contiguous relations	224

12.3. A miscellany of results on π	228
12.4. New generating functions	233
12.5. Series for $1/\pi$ using Legendre's relation	238
Chapter 13. Weighted Sum Formulas for Multiple Zeta Values	253
13.1. Introduction	253
13.2. Elementary proofs	254
13.3. New sums	256
13.4. More sums from recursions	265
13.5. Length 3 and higher multiple zeta values	272
13.6. Another proof of Zagier's identity	279
Chapter 14. Further Applications of Experimental Mathematics	283
14.1. Contiguous relations	283
14.2. Orthogonal polynomials	293
14.3. Gaussian quadrature	301
Bibliography	307

CHAPTER 0

Introduction

Abstract. In the first quarter of this dissertation, we investigate the problem of how far a walker travels after n unit steps, each taken along a uniformly random direction; the short-step behaviour of this random walk was unknown. Utilising functional equations, we fully analyse the three- and four-step walks, finding the moments and densities of the distance from the origin. Our methods involve a blend of combinatorics, probability, and complex analysis.

The derivatives of random walk moments turn out to be Mahler measures. We fruitfully study them using elementary techniques (different to those used by other researchers), namely generating functions of log-sine integrals and trigonometry. On the other hand, some random walk moments can be written as moments of products of complete elliptic integrals. These are studied, culminating in a complete solution for the moments of the product of two elliptic integrals. We also give some results when more elliptic integrals are involved. These endeavours occupy the second quarter of this dissertation.

A spectacular application of elliptic integrals is their ability to produce rational series which converge to $1/\pi$, as observed by Ramanujan. Using modular forms and hypergeometric transforms, we produce new classes of $1/\pi$ series which involve Legendre polynomials and Apéry-like sequences. We give a diverse range of series for related constants, including some based on Legendre's relation. The third quarter of this dissertation is devoted to this topic.

In the last quarter we apply experimental methods to better understand a number of areas encountered in our prior investigations. We simplify proofs for some multiple zeta value identities, give new ones and outline how they may be found. We give a method to quickly generate contiguous relations for hypergeometric series. Lastly, we look at orthogonal polynomials, in particular a new application of Gaussian quadrature to multi-dimensional lattice sums.

0.1. Acknowledgments

I would like to thank my supervisors, Jonathan Borwein and Wadim Zudilin, for their tireless efforts and enormous patience, for sharing with me many ideas and opportunities, and for introducing me to the world of research. Their scholarly expertise and dedication to students are the main reasons I chose to study at the University of Newcastle.

I would also like to thank my other coauthors, David Borwein, Heng Huat Chan, Lawrence Glasser, Dirk Nuyens, Mathew Rogers, Armin Straub, and John Zucker, who have provided me with immense help and support, and whose work contribute to part of this dissertation. Special thanks goes to Armin Straub, with whom I have shared an office on several occasions, and I have benefited greatly from our conversations.

I am grateful to my thesis examiners; their careful reading and subsequent comments improved this dissertation. Any errors that remain are entirely mine.

Finally, I would like to thank Kate Mulcahy for her unfailing support.

0.1.1. The chapters. The bulk of **Chapter 1** is based on the published paper [53],

J. M. Borwein, D. Nuyens, A. Straub and J. G. Wan, Some arithmetic properties of short random walk integrals, *Ramanujan Journal* **26** (2011), 109–132.

We are grateful to David Bailey, David Broadhurst and Richard Crandall for helpful suggestions, to Bruno Salvy and Michael Mossinghoff for pointing us to crucial references, and to Peter Donovan for stimulating this research.

Some of the more significant new results include Proposition 1.1, remarks 1.2.1–1.2.2, Theorem 1.2, Theorem 1.4 and example 1.5.1 (they are *new in the sense that* the results are unknown prior to the work [53]).

Chapter 2 is mostly based on the published paper [56],

J. M. Borwein, A. Straub and J. G. Wan, Three-step and four-step random walk integrals, *Experimental Mathematics*, **22** (2013), 1–14.

We are grateful to Wadim Zudilin for useful discussions, and for pointing out a number of references, which have been crucial in obtaining the closed forms in the paper.

Some of the new results include Propositions 2.1–2.2, Theorems 2.2–2.6, remarks 2.2.2–2.3.2, corollary 2.2, examples 2.3.1–2.3.2 and subsection 2.3.1.

Chapter 3 is largely adapted from the published paper [57],

J. M. Borwein, A. Straub, J. G. Wan and W. Zudilin, with an appendix by D. Zagier, Densities of short uniform random walks, *Canadian Journal of Mathematics* **64** (2012), 961–990.

We are grateful to David Bailey for numerical assistance, Michael Mossinghoff for pointing us to the Mahler measure conjectures, and Plamen Djakov and Boris Mityagin for correspondence related to a theorem. We are especially grateful to Don Zagier for pointing out proofs of a former conjecture, and for helpful comments and improvements.

Some of the new results are Theorem 3.1, examples 3.3.1–3.3.2, Theorem 3.4–3.8, and Sections 3.6–3.7. Equation (3.21) is a new addition (*in the sense that it is not in the paper the chapter is based on, being added later*).

Chapter 4 has not appeared in print.

I have not been able to find the majority of the results from Section 4.2 onwards in the literature, and hence believe them to be new, though some of them are not particularly difficult to produce. Theorem 4.1, Theorem 4.4 and example 4.3.5 may be of some interest.

Chapter 5 is heavily edited from the published paper [40],

D. Borwein, J. M. Borwein, M. L. Glasser and J. G. Wan, Moments of Ramanujan’s generalized elliptic integrals and extensions of Catalan’s constant, *Journal of Mathematical Analysis and Applications* **384** (2011), 478–496.

We want to thank Roberto Tauraso for posing a question which led to this research.

Some of the new results presented in this work include Theorem 5.3 (and its proof and subsequent discussion), remark 5.2.1, Theorems 5.5–5.7, and Proposition 5.1.

Chapter 6 is based on my published paper [190],

J. G. Wan, Moments of products of elliptic integrals, *Advances in Applied Mathematics* **48** (2012), 121–141.

I wish to thank David Bailey for providing extensive tables showing relations of various integrals, and also to thank Jonathan Borwein, Lawrence Glasser and Wadim Zudilin for many helpful comments.

Some of the new results are stated at the end of Section 6.1; a number of results have also been added since publication, for instance equation (6.65).

Chapter 7 has not appeared in print and is solely my work, the exception being much of Section 7.9, which is my paraphrasing of the submitted joint article [169], M. Roger, J. G. Wan and I. J. Zucker, Moments of elliptic integrals and critical L -values, *preprint* (2013).

I would like to thank Lawrence Glasser and Wadim Zudilin for helpful discussions.

Much of the analysis is new, leading to Theorems 7.1–7.3, Proposition 7.1, and corollary 7.1. Several subsequent sections are also new; we highlight example 7.7.1, the proof in example 7.7.4, and Sections 7.8–7.10.

Chapter 8 is my own work; Section 8.4 comes from my contribution to the joint paper [41] (see below).

I thank Wadim Zudilin for inspiration, and Mat Rogers for pointing out many useful references.

Parts of the chapter are expository, though simplified proofs for some known results have been obtained in remark 8.1.2, equation (8.9), example 8.1.1, and Section 8.2. Section 8.3 has not been previously published; Section 8.4 (in particular Theorem 8.2) is new.

Chapter 9 is a significantly altered adaptation of the published paper [41],

D. Borwein, J. M. Borwein, A. Straub and J. G. Wan, Log-sine evaluations of Mahler measures, II, *Integers* **12A** (2012), #A5, 30 pages.

We thank David Bailey for his assistance with quadratures. Thanks are also due to Yasuo Ohno and Yoshitaka Sasaki for introducing us to the relevant papers.

New and improved results include example 9.2.1, example 9.2.3, example 9.5.2, subsection 9.5.2, and remark 9.6.1.

Most of **Chapter 10** is based on the published paper [74],

H. H. Chan, J. G. Wan and W. Zudilin, Legendre polynomials and Ramanujan-type series for $1/\pi$, *Israel Journal of Mathematics* (2012), published electronically, 25 pages.

Section 10.10 is based on the published paper [73],

H. H. Chan, J. G. Wan and W. Zudilin, Complex series for $1/\pi$, *Ramanujan Journal* 29 (2012), 135–144.

We would like to credit Zhi-Wei Sun for raising a new family of remarkable series for $1/\pi$.

The results in this chapter and the next, unless otherwise stated, are original (in the sense that they were first published in [74], [73] or [193]). Some materials in Sections 10.3 and 10.5 (e. g. remarks 10.3.1 and 10.5.2) have been added since publication and have not previously appeared.

Chapter 11 follows closely the published paper [193],

J. G. Wan and W. Zudilin, Generating functions of Legendre polynomials: a tribute to Fred Brafman, *Journal of Approximation Theory* 164 (2012), 488–503.

We are indebted to Peter Duren and Suzanne Rogers for Brafman’s biography information. We would also like to thank Richard Askey, Paul Goodey and Angela Startz for related comments and information. Special thanks are due to Heng Huat Chan whose advice and support have been crucial.

Chapter 12 has not appeared in print, with the exception of Section 12.5 which has been put on-line [191] (this manuscript has since been accepted by *Integral Transforms and Special Functions*).

I would like to thank Wadim Zudilin for his support during many stages of this project, and Heng Huat Chan for his helpful comments.

Section 12.1 contains new results (e. g. equations (12.4), (12.8)) and simplified proofs of known results (e. g. equation (12.7)). Section 12.2 contains constructions probably not explored previously. Section 12.3 summarises some known techniques, and also proves a number of new results (stated at the start of the section); of note are Theorems 12.2–12.4. Section 12.5 is entirely new, and provides alternative proofs for some earlier series.

The first 4 sections of Chapter 13 are based on my paper [192],

J. G. Wan, Some notes on weighted sum formulae for double zeta values. *Number Theory and Related Fields, in memory of Alf van der Poorten*, in: Springer Proceedings in Mathematics & Statistics **43** (2013), 361–379.

I wish to thank John Zucker and Wadim Zudilin for illuminating discussions, and Yasuo Ohno for pointing out a reference. I am extremely grateful to Wadim Zudilin who actually typeset the first version of Section 13.6.

Section 13.2 gives shorter proofs of known identities. Sections 13.3–13.4 are original. Section 13.5 first provides simpler proofs of known results (of note is remark 13.5.2), then proceeds to give a number of new ones, such as Propositions 13.3–13.5, Theorem 13.7 and Lemma 13.2. Section 13.6 gives a neater proof of a recent theorem. The last 2 sections have not previously appeared in print.

Chapter 14 has not appeared in print, except that a very brief and edited summary of Section 14.3 will appear in the book [52],

J. M. Borwein, R. C. McPhedran, M. L. Glasser, J. G. Wan and I. J. Zucker, *Lattice Sums Then and Now*, in: Encyclopedia of Mathematics and its Applications, **150**, Cambridge University Press, to appear August 2013, ~380 pages.

I am grateful to O-Yeat Chan for much help and discussions, and for his draft and summary of ideas for the material on Gaussian quadrature.

Section 14.1 unifies several known approaches and gives new ones, thus simplifying proofs of many contiguous relations. Section 14.2 gives a new way to look at some orthogonal polynomials and produces some identities. Section 14.3 introduces the new idea of using Gaussian quadrature to approximate multiple sums.

0.2. Overview

0.2.1. Experimental mathematics. This dissertation explores a range of related topics in number theory and special functions, starting from investigations of uniform random walks on the plane, using techniques from *experimental mathematics* where possible. As such, it is not an attempt to solve a single difficult problem nor does it try to develop a unified theory. Each chapter contains new results discovered and proven experimentally, facilitated by the computer.

Modern experimental mathematics [21, 43, 44] seeks to fully utilise the computer's capability beyond mere calculations and simulations. More thoughtful control of the computer allows one to use graphics to suggest underlying mathematical principles, test and falsify conjectures, and confirm analytical results. Intelligent experiments allow the computer to help us gain intuition and insight, discover new patterns, and suggest approaches for proofs.

Two strands of algorithms are prominent in experimental mathematics. The first is creative telescoping, which achieves automatic evaluation of many sums and integrals, in particular sums involving binomial coefficients. Its long lineage of algorithms starts with Celine, followed by Gosper and then Wilf-Zeilberger (WZ), and more are still being actively developed and refined. Both Celine's and the WZ algorithm attempt to find a recursion in n for the sum $F(n) := \sum_{k=a}^n a(n, k)$, while Gosper's algorithm tries to write $a(n, k)$ as $b(n, k+1) - b(n, k)$, making the sum into a telescoping one (and providing a proof if no b exists).

Thus, a typical proof of a sum identity $\sum_{k=a}^n a(n, k) = R(n)$ in experimental mathematics looks like this: apply a suitable algorithm to find a recursion satisfied by the left hand side; check that the right hand side satisfies the same recursion; check enough initial conditions and conclude the the two sides are equal. By the same token, a proof of an identity between analytic functions would involve producing a differential equation for one side (if this side is a generating function, then a differential equation can come from a recursion satisfied by the coefficients), checking that the other side is annihilated by the differential equation, and checking some initial conditions. We will use these approaches time and again.

The other strand involves reverse engineering, and outstanding examples include the PSLQ and LLL algorithms. PSLQ takes an input vector v of real numbers, and attempts to find an integer vector u , such that $v \cdot u = 0$ within the prescribed precision. If no u is found, it can certify that no such vector below a certain norm exists. PSLQ can be used when trying to write a numerically computed answer in terms of supplied, well-known constants, or as the root of a polynomial. Often, knowing a closed form answer brings one much closer to a proof. Moreover, in many cases once an answer is found, it can be easily proved, though finding the answer can be computationally expensive; in these instances PSLQ can be used to

replace analytical computations and arrive at a checkable answer more efficiently. We adhere to this practice often.

The very nature of experimental mathematics lends itself to problem solving. It is also conducive to interdisciplinary research, in particular with sciences wherein traditional experimentation is deeply entrenched. These strengths are hopefully reflected in the diverse background of problems presented, investigated, and solved here. Additionally, experimental methods tend to reduce formerly difficult analysis to much simpler algebra, for instance creative telescoping uses not much more than linear algebra, but unifies proofs previously requiring much ingenuity. In the same spirit, we try to give elementary proofs of results whenever possible.

0.2.2. Notations. Throughout, we will use the standard notation for the generalised hypergeometric series,

$${}_pF_q \left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \middle| z \right) = \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_p)_n}{(b_1)_n \cdots (b_q)_n} \frac{z^n}{n!},$$

where $(a)_n = \Gamma(a+n)/\Gamma(a)$ is the Pochhammer symbol, and $\Gamma(z)$ is the Gamma function. Generalised hypergeometric series provide a framework which unifies many binomial sums and special functions. In particular, ${}_2F_1$'s and ${}_3F_2$'s enjoy many transformations and exhibit rich structures. By saying that an expression has a closed form, we mean that it can be written in terms of hypergeometric series and well-known constants (such as π).

Two Gaussian hypergeometric functions (${}_2F_1$'s) which receive our special attention are the elliptic integrals of the first and second kinds, given respectively by

$$K(x) = \frac{\pi}{2} {}_2F_1 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| x^2 \right) = \int_0^{\pi/2} \frac{dt}{\sqrt{1-x^2 \sin^2 t}},$$

$$E(x) = \frac{\pi}{2} {}_2F_1 \left(\begin{matrix} -\frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| x^2 \right) = \int_0^{\pi/2} \sqrt{1-x^2 \sin^2 t} dt.$$

We also denote the complementary modulus $\sqrt{1-x^2}$ by x' , and use $K'(x) := K(x')$, $E'(x) := E(x')$. We denote the p th singular value of K by k_p : that is, k_p is the unique real number satisfying $K'(k_p)/K(k_p) = \sqrt{p}$. It is known that when p is a natural number, k_p is algebraic and effectively computable, see [46, 175, 206].

The Riemann zeta function is given, for $\operatorname{Re} s > 1$, by

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s},$$

and can be analytically continued to the whole complex plane except for the simple pole at $s = 1$.

When an equality is only conjectural (for instance, based on numerical evidence), we indicate it using the symbol $\stackrel{?}{=}$.

Other notations will be introduced in the chapters as they appear.

0.2.3. Random walks. The first four chapters of this dissertation are concerned with random walks; specifically, we investigate the century-old problem of how far a random walker travels after n steps, each step being of unit length and taken along a uniformly random direction in the plane. Such walks date back to Rayleigh and Pearson, and find applications in modeling Brownian motion, superposition of waves, quantum chemistry, and migration of organisms.

While the asymptotics of this walk were understood, the short-step behaviour was not known – such was the impetus for us to embark on this study. Denoting the s th moment of the distance from the origin of the n -step walk by $W_n(s)$, and the radial probability density by $p_n(x)$, we have

$$W_n(s) = \int_0^n x^s p_n(x) dx = \int_{[0,1]^n} \left| \sum_{k=1}^n e^{2\pi i x_k} \right|^s d\mathbf{x}. \quad (0.1)$$

In Chapter 1, we first gain intuition using numerical integration, which allows us to combinatorially deduce the even moments:

$$W_n(2k) = \sum_{a_1 + \dots + a_n = k} \binom{k}{a_1, \dots, a_n}^2. \quad (0.2)$$

The recursion in k satisfied by the right hand side gives us a recurrence relation for $W_n(2k)$, which lifts to a functional equation by Carlson's theorem. This lets us analytically continue $W_n(s)$ to the complex plane with poles at certain negative integers; the poles are crucial to our understanding of p_n via techniques such as the Mellin transform.

Inspired by a combinatorial convolution satisfied by (0.2), we conjecture

$$W_{2n}(s) \stackrel{?}{=} \sum_{j \geq 0} \binom{s/2}{j}^2 W_{2n-1}(s-2j), \quad (0.3)$$

which is used in numerical checks, and is a driving force for subsequent chapters. The conjecture holds when s is an even positive integer, and when $n = 1$.

While it is easy to find

$$p_2(x) = \frac{2}{\pi\sqrt{4-x^2}}, \quad W_2(s) = \binom{s}{s/2}, \quad (0.4)$$

a closed form formula for $W_3(s)$ involves more effort. Our result is in terms of the generalised hypergeometric series: for integer k ,

$$W_3(k) = \operatorname{Re} {}_3F_2\left(\begin{matrix} \frac{1}{2}, -\frac{k}{2}, -\frac{k}{2} \\ 1, 1 \end{matrix} \middle| 4\right). \quad (0.5)$$

To prove this, we take a typical approach in experimental mathematics. Using creative telescoping, we show that both sides satisfy the same three-term recurrence, and therefore we only need to prove the identity for $k = \pm 1$. This is accomplished using some classical analysis, in particular transformation formulas for the complete elliptic integrals K and E . As a consequence, we were the first to discover the expected distance for the 3-step walk,

$$W_3(1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4} \frac{2^{2/3}}{\pi^4} \Gamma^6\left(\frac{2}{3}\right), \quad (0.6)$$

as well as

$$W_3(-1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right). \quad (0.7)$$

In Chapter 2, we manage to express both $W_3(s)$ and $W_4(s)$ in terms of Meijer G -functions, and then as hypergeometric functions. A careful analysis using these special functions gives the new result

$$W_4(-1) = \frac{\pi}{4} {}_7F_6\left(\begin{matrix} \frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{1}{4}, 1, 1, 1, 1, 1 \end{matrix} \middle| 1\right), \quad (0.8)$$

and a closed form for $W_4(1)$ as the sum of two ${}_7F_6$'s. Together they give all the integer moments of the 4-step walk. Using conditional probability, we ultimately deduce that

$$W_4(-1) = \frac{8}{\pi^3} \int_0^1 K^2(k) dk = \frac{4}{\pi^3} \int_0^1 K'(k)^2 dk. \quad (0.9)$$

Moreover, we find the series expansion for p_3 and the poles of $W_3(s)$, all in terms of $W_3(2k)$. Various connections with Bessel functions are given.

While p_3 was known as the real part of a function involving K , p_4 was unknown before our work. Shifting focus to the densities, in Chapter 3 we give the beautiful

formulas

$$p_3(x) = \frac{2\sqrt{3}}{\pi} \frac{x}{(3+x^2)} {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \middle| \frac{x^2(9-x^2)^2}{(3+x^2)^3}\right), \quad (0.10)$$

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16-x^2}}{x} \operatorname{Re} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{(16-x^2)^3}{108x^4}\right). \quad (0.11)$$

The first formula is inspired by a functional equation we found for p_3 , itself a serendipitous discovery. A careful analysis of p_4 using asymptotics, pole structures, and differential equations allows us to write down the second formula, which admits a modular parametrisation. We also find the first residue of W_5 .

To complete our analysis of three and four step walks (where all our closed forms are new), we again appeal to Carlson's theorem and existing literature on Bessel functions to give a single hypergeometric form for $W_3(s)$ where s is not a negative integer less than -1 :

$$W_3(s) = \frac{3^{s+3/2}}{2\pi} \frac{\Gamma(1+s/2)^2}{\Gamma(s+2)} {}_3F_2\left(\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2} \middle| \frac{1}{4}\right). \quad (0.12)$$

This is done by recasting W_3 as integrals of modified Bessel functions. A formula where s is a negative integer is also found. We also give a single Meijer G representation for $W_4(s)$, valid for all s :

$$W_4(s) = \frac{2^{2s+1}}{\pi^2 \Gamma(\frac{1}{2}(s+2))^2} G_{4,4}^{2,4}\left(\begin{matrix} 1, 1, 1, \frac{s+3}{2} \\ \frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2}, \frac{1}{2} \end{matrix} \middle| 1\right). \quad (0.13)$$

Finally, we are able to give a proof of the conjecture (0.3) for $n = 2$ and s an integer.

In Chapter 4, we look at a number of related problems. The first is the average displacement of a 3-step walk with step sizes $1, 1, a$. When $a = 2$, the average is $\frac{48\pi}{\Gamma(1/4)^4} + \frac{\Gamma(1/4)^4}{4\pi^3}$. The second problem involves an elementary derivation of $p_3(x)$. Thirdly we look at some random walks in higher dimensions; dimension 3 is particularly easy and we find all the densities. We also look at some asymptotic behaviour. Finally, we study random walks in the plane with restricted numbers of directions, and find a curious phenomenon where some even moments of distances traveled for these walks agree exactly with the moments of the uniform random walk. Many of the results in this chapter have not appear previously in print.

0.2.4. Elliptic integrals. The ubiquitous appearance of the complete elliptic integrals in random walks (such as equation (0.9)) leads us to a full study of the moments of these integrals. Complete elliptic integrals first appeared in the exact

expression for the period of a pendulum and the perimeter of an ellipse, but since then have found applications in diverse pure and applied areas. In Chapter 5, we revise some basic properties satisfied by the complete elliptic integrals (such as Legendre's relation), and use standard techniques to compute in closed form integrals involving a single E or K , as well as their hypergeometric generalisations K^s and E^s . We give many closed forms, including a class of constants which are good candidates for being generalisations of Catalan's constant, expressible in terms of the digamma function; here contour integration, Carlson's theorem, and other standard techniques are recalled and used. We also include a range of ${}_3F_2$ identities.

In Chapters 6 and 7, we use a variety of strategies to give closed form evaluations of integrals, where the integrands involve (mostly products of) the elliptic integrals K , K' , E and E' . The strategies include interchanging the order of summation and integration, using the quadratic transformations of E and K , appealing to a Fourier series, applying Legendre's relation, integrating by parts, and using a result of Zudilin that converts certain triple integrals into ${}_7F_6$'s.

In Chapter 6, we give explicit proofs that the odd moments of K'^2 , E'^2 , $K'E'$, K^2 , E^2 and KE can be written as $a+b\zeta(3)$, with $a, b \in \mathbb{Q}$, while the odd moments of $K(x)K'(x)$, $E(x)K'(x)$, $K(x)E'(x)$ and $E(x)E'(x)$ are rational linear combinations of π and π^3 . We use techniques in experimental mathematics to give recursions satisfied by the moments of those functions, and to prove results such as

$$\int_0^1 \frac{x}{1-t^2x^2} K(x)K'(x) dx = \frac{\pi}{4} K(t)^2.$$

We derive the Fourier series for $K(\sin t)$ and $E(\sin t)$ along with some applications, and give many equivalent integral formulations of $W_4(-1)$ in Theorem 6.4.

In Chapter 7, we more fruitfully study integrals of the form $\int_0^1 G(x)(1+x)^n dx$. Our main result is elegant, and states that for $n \in \mathbb{Z}$ and G a product of up to two elliptic integrals, $\int_0^1 G(x)(1+x)^n dx$ can be written as a \mathbb{Q} -linear combination of elements taken from the set

$$\{1, \pi, \pi^2, \pi^3, \pi \log 2, G, \zeta(3), A, B, C, D\},$$

where A, B, C, D are hypergeometric series defined there and G is Catalan's constant studied before. In particular, this implies all moments of the product of two

elliptic integrals can all be expressed in closed form, and thus any linear relationship between them (first observed by Bailey and Borwein) can be routinely verified.

In the same chapter we record a number of sporadic integrals of varying generality (many are original), give a list of indefinite integrals with closed forms, and discover a hypergeometric transform. Manipulations of hypergeometric series feature more heavily in this chapter, for instance the following identity implicitly involves closed form hypergeometric evaluations:

$$\int_0^1 \left(\frac{x}{x'}\right)^{\frac{1}{2} \pm \frac{1}{4}} K(x) dx = \frac{\pi^2}{12} \sqrt{5 \pm \frac{1}{\sqrt{2}}}.$$

We resolve some experimental observations raised in the previous chapter regarding the integral of K^3 . Using Fourier series, θ functions, and lattice sums, we give the first closed form evaluation of the cube of an elliptic integral:

$$\int_0^1 K'(x)^3 dx = 3 \int_0^1 K(x)^2 K'(x) dx = 5 \int_0^1 x K'(x)^3 dx = \frac{\Gamma^8(1/4)}{128\pi^2}. \quad (0.14)$$

Combined with Legendre's relation, we also evaluate other integrals involving the product of three elliptic integrals. On the other hand, such evaluations are intimately connected with L -values of modular forms, and provide new results on lattice sums, such as

$$\sum_{(m,n) \neq (0,0)} \frac{(-1)^{m+n} m^2 n^2}{(m^2 + n^2)^3} = \frac{\Gamma^8(1/4)}{2^9 3 \pi^3} - \frac{\pi \log 2}{8}.$$

0.2.5. Mahler measures. While investigating moments of random walks as analytic objects in the first four chapters, it became natural to ask for the derivatives of the moments, $W'_n(s)$. What we obtain are examples of Mahler measures of a polynomial, studied extensively in number theory via techniques dissimilar to ours. In particular, we give elementary computations for $W'_3(0) = \frac{1}{\pi} \text{Cl}\left(\frac{\pi}{3}\right)$ and $W'_4(0) = \frac{7}{2} \frac{\zeta(3)}{\pi^2}$ (here Cl denotes the Clausen function), which turned out to be classical evaluations of higher Mahler measures.

For k polynomials in n variables, the multiple higher Mahler measure is defined by

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

The connection with random walks is that

$$W_n^{(m)}(0) = \mu_m(1 + x_1 + \dots + x_{n-1}),$$

where $\mu_m(P) = \mu(P, \dots, P)$ with P repeated m times. In Chapter 8, we collect some basic facts, evaluation techniques and conjectures about Mahler measures, in particular the powerful Jensen's formula, and a closely related trigonometric version which seems more versatile:

$$\int_0^1 \log |2a + 2b \cos(2\pi x)| dx = \log (|a| + \sqrt{a^2 - b^2}), \quad |a| \geq |b| > 0. \quad (0.15)$$

The formula leads to a quick proof of two of Boyd's conjectures, namely

$$\begin{aligned} \mu(y^2(x+1)^2 + y(x^2 + 6x + 1) + (x+1)^2) &= \frac{16G}{3\pi}, \\ \mu(y^2(x+1)^2 + y(x^2 - 10x + 1) + (x+1)^2) &= \frac{20}{3\pi} \text{Cl}\left(\frac{\pi}{3}\right), \end{aligned}$$

while finding a new evaluation. Many classical results, such as $\mu(a + bx + cy)$ and $\mu((2 \sin s)^n + (x + y)^n)$, can all be found using (0.15).

In the same chapter, we give an elementary evaluation of $\mu_k = \mu(k + x + 1/x + y + 1/y)$, and using integrals of K , produce a functional equation for this Mahler measure in terms of k , recovering results such as $2\mu_5 = \mu_1 + \mu_{16}$. We also use elementary methods to reduce $\mu((1+x)(1+y) + z)$ to a single integral, thereby confirming another of Boyd's conjectures numerically to 1000 digits.

In Chapter 9, we find that many Mahler measures can be expressed in terms of log-sine integrals, studied for instance by Lewin. Some classes of log-sine integrals conveniently have very nice generating functions, which means certain Mahler measures can be computed easily (in fact, entirely symbolically).

We fruitfully apply the epsilon expansion technique borrowed from physics, to find an expression for $\mu_2(1 + x + y)$ in terms of a log-sine integral, namely

$$\mu_2(1 + x + y) = \frac{3}{\pi} \text{Ls}_3\left(\frac{2\pi}{3}\right) + \frac{\pi^2}{4}. \quad (0.16)$$

We also give a conjectural closed form for $\mu_3(1 + x + y)$. We then digress into combinatorics, and produce a sequence of results coming from a blend of enumeration and trigonometry, which pave the way for potentially useful analysis of some higher Mahler measures, including $\mu_2(1 + x + y)$. In doing so, we also produce closed forms for multiple polylogarithms of low weights. The technique used in the last part is essentially the shuffle relation of the multiple zeta values, which we come back to in Chapter 13.

In Section 9.6, we give a third, and more analytical evaluation of $\mu_2(1 + x + y)$.

0.2.6. Series for $1/\pi$. The functions E^s and K^s studied in Chapter 5 are crucial in proving Ramanujan's original series for the transcendental constant $1/\pi$. In Chapter 10, we investigate a new type of Ramanujan-type series first conjectured by Sun. Such series take the form

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} (A + Bn) P_n(x_0) z_0^n = \frac{C}{\pi},$$

where $s \in \{1/2, 1/3, 1/4, 1/6\}$, $P_n(x)$ denotes the Legendre polynomial, and frequently the summands are rational numbers.

In order to prove such new series, we appeal to an all-but-forgotten generating function due to Brafman,

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} P_n(x) z^n = {}_2F_1\left(s, 1-s \mid \frac{1-\rho-z}{2}\right) \cdot {}_2F_1\left(s, 1-s \mid \frac{1-\rho+z}{2}\right), \quad (0.17)$$

where $\rho = (1 - 2xz + z^2)^{1/2}$. Writing the ${}_2F_1$ as F , Brafman's formula assumes the form

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} P_n(x) z^n = F(\alpha)F(\beta).$$

We notice that when α and β are related by a modular equation, namely, $\alpha = t(\tau_0)$ and $\beta = t(\tau_0/N)$, where t is a suitable modular function, then the right hand side of (0.17) can be written in terms of $F^2(\alpha)$ and its z -derivative in terms of $F(\alpha)F'(\alpha)$. These two terms can be related, by Clausen's formula, to building blocks of the classical Ramanujan series,

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n(s)_n(1-s)_n}{n!^3} (a + bn)(4\alpha(1-\alpha))^n = \frac{c}{\pi},$$

for which we have a well-developed theory. Therefore, all of Sun's conjectures are reduced to classical Ramanujan series and proven. We provide detailed calculations, and give many more new series and their 'companions'. A range of other techniques, involving hypergeometric transformations and singular values of K , are also presented. An example of a new series with rational summands is

$$\sum_{n=1}^{\infty} \frac{(\frac{1}{4})_n(\frac{3}{4})_n}{n!^2} (841 + 9520n) P_n\left(\frac{4097}{4095}\right) \left(\frac{455}{29241}\right)^n = \frac{513\sqrt{114}}{2\pi},$$

and a connection between rational series and class numbers is observed.

In Section 10.10, we give a heavily modular method to produce complex series for $1/\pi$ which are rarer but have been observed in our work. A number of other complex series are included.

In Chapter 11, we continue our study of $1/\pi$ series and Legendre polynomials, by first giving a very general generating function,

$$\begin{aligned} & \sum_{n=0}^{\infty} u_n P_n \left(\frac{(X+Y)(1+cXY) - 2aXY}{(Y-X)(1-cXY)} \right) \left(\frac{Y-X}{1-cXY} \right)^n \\ &= (1-cXY) \left\{ \sum_{n=0}^{\infty} u_n X^n \right\} \left\{ \sum_{n=0}^{\infty} u_n Y^n \right\}, \end{aligned} \quad (0.18)$$

where u_n is an Apéry-like sequence, satisfying $(n+1)^2 u_{n+1} = (an^2 + an + b)u_n - cn^2 u_{n-1}$, $u_{-1} = 0$ and $u_0 = 1$. We find it significant that both the statement and the proof of the generating function were found with the help of computers. Manipulating (0.18) gives generating functions for rarefied Legendre polynomials, for instance

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} P_{2n} \left(\frac{(X+Y)(1-XY)}{(X-Y)(1+XY)} \right) \left(\frac{X-Y}{1+XY} \right)^{2n} \\ &= \frac{1+XY}{2} {}_2F_1 \left(\frac{1}{2}, \frac{1}{2} \mid 1-X^2 \right) {}_2F_1 \left(\frac{1}{2}, \frac{1}{2} \mid 1-Y^2 \right). \end{aligned} \quad (0.19)$$

We are thus able to find new series for $1/\pi$ whose summands involve Apéry-like sequences or rarefied Legendred polynomials, examples of which include

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} (2+15n) P_{2n} \left(\frac{3\sqrt{3}}{5} \right) \left(\frac{2\sqrt{2}}{5} \right)^{2n} = \frac{15}{\pi}, \\ & \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} (1+9n) P_{3n} \left(\frac{4}{\sqrt{10}} \right) \left(\frac{1}{\sqrt{10}} \right)^{3n} = \frac{\sqrt{15+10\sqrt{3}}}{\pi\sqrt{2}}, \\ & \sum_{n=0}^{\infty} \left\{ \sum_{k=0}^n \sum_{j=0}^k \binom{n}{k} \left(\frac{-1}{8} \right)^k \binom{k}{j}^3 \right\} n P_n \left(\frac{5}{3\sqrt{3}} \right) \left(\frac{4}{3\sqrt{3}} \right)^n = \frac{9\sqrt{3}}{2\pi}. \end{aligned}$$

In Chapter 12, we first investigate some other consequences of Brafman's formula and their implications for special functions. We describe the Borweins' approach for producing $1/\pi$ series, and summarise some other methods used, in particular hypergeometric summation formulas and Fourier-Legendre expansion. We also use contiguous relations (studied later) to analyse some closely related series. Next, using a new class of generating functions shown using the Wilf-Zeilberger

algorithm, we prove many more conjectured series for $1/\pi$. An example of a new generating function is

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{2n-2k}{n-k} \binom{2k}{k}^2 \binom{2n}{n} \frac{x^{k+n}}{(1+4x)^{2n+1}} = {}_3F_2 \left(\begin{matrix} \frac{1}{3}, \frac{1}{2}, \frac{2}{3} \\ 1, 1 \end{matrix} \middle| 108x^2(1-4x) \right),$$

and we also discuss their curious ‘satellite identities’.

The last part of Chapter 12 introduces the new idea of proving $1/\pi$ series using only Legendre’s relation and (simple) modular transforms. The calculations are very involved, albeit elementary. We discover an unusual formula,

$$\sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n \left(\frac{1}{2} \right) \left(\frac{3}{128} \right)^n (3+14n) = \frac{8\sqrt{2}}{\pi},$$

which cannot be explained by the general theory of Chapter 10, but also recover many classical Ramanujan series, such as

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{6})_n (\frac{1}{2})_n (\frac{5}{6})_n}{n!^3} \left(\frac{4}{125} \right)^n (1+11n) = \frac{5\sqrt{15}}{6\pi},$$

thereby suggesting that our approach may provide an alternative route to those series. Lastly, we use Orr-type theorems to give series that converge to other well-known constants.

0.2.7. Multiple zeta values. Multiple zeta values are special values of the multiple polylogarithm studied in Chapter 9. In Chapter 13, we give a unified and elementary approach for studying sum formulas for double zeta values, defined by

$$\zeta(a, b) = \sum_{n=1}^{\infty} \sum_{m=1}^{n-1} \frac{1}{n^a m^b},$$

as well as the alternating versions of these sums (replacing the 1 in the numerator by, say, $(-1)^m$), and finally sums where the numerators are replaced by Dirichlet characters.

In particular, we find the first elementary proof of an identity by Ohno and Zudilin,

$$\sum_{j=2}^{s-1} 2^j \zeta(j, s-j) = (s+1)\zeta(s), \quad (0.20)$$

as discover its alternating companion,

$$\sum_{j=2}^{s-1} 2^j \zeta(\bar{j}, s-j) = (3-2^{2-s}-s)\zeta(s). \quad (0.21)$$

Moreover, we give some new results for the Mordell-Tornheim double sums, and use a generating function approach to prove a new evaluation involving the harmonic numbers H_n ,

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{H_n}{(2n+1)^{2s-1}} &= (1-4^{-s})(2s-1)\zeta(2s) - (2-4^{1-s})\log(2)\zeta(2s-1) \\ &\quad + (1-2^{-s})^2\zeta(s)^2 - \sum_{k=2}^s 2(1-2^{-k})(1-2^{k-2s})\zeta(k)\zeta(2s-k). \end{aligned}$$

We showcase a number of experimental methods. For instance, an experimental approach can be used to discover or to rule out sum identities for the double zeta values. Then, using recursions of the Riemann zeta function, we prove new sum identities such as

$$\begin{aligned} &\sum_{j=2}^{n-2} (j-1)(2j-1)(n-j-1)(2n-2j-1)\zeta(2j, 2n-2j) \\ &= \frac{3}{8}(n-1)(3n-2)\zeta(2n) - 3(2n-5)\zeta(4)\zeta(2n-4). \end{aligned} \quad (0.22)$$

In Section 13.5, we prove some of the recursions used earlier in the chapter, plus some others which involve the product of three or more zeta terms. Using these, we give elementary proofs of summation formulas for weight 3, 4 and 5 multiple zeta values. Some of our results are new, the most interesting example being

$$\sum_{a+b+c+d+e=n} \zeta(2a, 2b, 2c, 2d, 2e) = \frac{945}{16}\zeta(2n) - \frac{315}{8}\zeta(2)\zeta(2n-2) + \frac{45}{8}\zeta(4)\zeta(2n-4).$$

To prove the above sum, we need a new ζ convolution identity which was first discovered experimentally. Results such as the above, where the right hand side is a rational multiple of π^{2n} , also exist in higher dimensions.

In the last section of Chapter 13, we simplify the proof of an involved evaluation of a multiple zeta value given by Zagier. The simplification maximises the use of experimental techniques (here, Gosper's algorithm), which results in minimal analyses being required.

0.2.8. Further applications. Applications of experimental mathematics to classical and new fields are by no means limited to some of the chapters we have investigated so far. In Chapter 14, we describe two useful tools that are easily implemented using computer algebra systems (CAS). The first concerns *contiguous relations*, that is, linear relations among hypergeometric series whose parameters

differ by integers. The method presented here allows us to check and generate all the contiguous relations required in the previous chapters. We prove a theorem which states that any series contiguous to F can be expressed as a linear combination of F and its derivatives. While the result was essentially known to Bailey, we take advantage of the speed of modern computers and the PSLQ algorithm to rapidly produce said linear combinations. The resulting contiguous relations can be used, for instance, to produce some new $1/\pi$ formulas in Chapter 12.

We also collect and derive many contiguous versions of the classical hypergeometric summation theorems in this Chapter, namely the theorems of Gauss, Kummer, Bailey, Saalschütz, Dixon, Watson and Whipple. Some of these results are previously known but scattered in the literature, moreover most are not yet implemented in computer algebra systems.

The second part of Chapter 14 deals with Gaussian quadrature, a general method that uses orthogonal polynomials to approximate integrals. Gaussian quadrature has been used to numerically check several sums and integrals encountered in the other chapters. We recap some basic results in the area, and give an account of a recent development where Gaussian quadrature (applied to a discrete measure) can be used to approximate infinite sums. We give an experimental method to rediscover, from scratch, some well-known orthogonal polynomials and their properties, complementing the heavy role that orthogonal polynomials played in our earlier chapters.

We then develop a new approach, which uses multiple Gaussian quadrature for summing over orthogonal rational functions. This approach lends itself unexpectedly well to the numerical evaluation of lattice sums, giving excellent results for a wide class of sums which previously could only be approximated using some levels of ingenuity. For example, we can obtain around 1.4 correct digits per weight used for the famous Madelung constant.

CHAPTER 1

Arithmetic Properties of Short Random Walk Integrals

ABSTRACT. We study the moments of the distance from the origin for a walk in the plane with unit steps in random directions. Our interest lies in closed forms for the moment functions and their values at the integers for a small number of steps. A closed form is obtained for the average distance traveled in three steps. This evaluation and its proof rely on combinatorial properties, such as recurrence equations of the even moments (which are lifted to functional equations). A general conjecture for even length walks is made.

1.1. Introduction, history and preliminaries

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

$$W_n(s) := \int_{[0,1]^n} \left| \sum_{k=1}^n e^{2\pi i x_k} \right|^s d\mathbf{x} \quad (1.1)$$

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 1. As such, the integral (1.1) 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 $W_n(1)$, the expected distance after n steps.

While the general structure of the moments and densities of the random walks studied here is understood 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 (1.14) and (1.30)), 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 1.5 that

$$W_3(1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4} \frac{2^{2/3}}{\pi^4} \Gamma^6\left(\frac{2}{3}\right) \quad (1.2)$$

where Γ is the *Gamma function* [11].

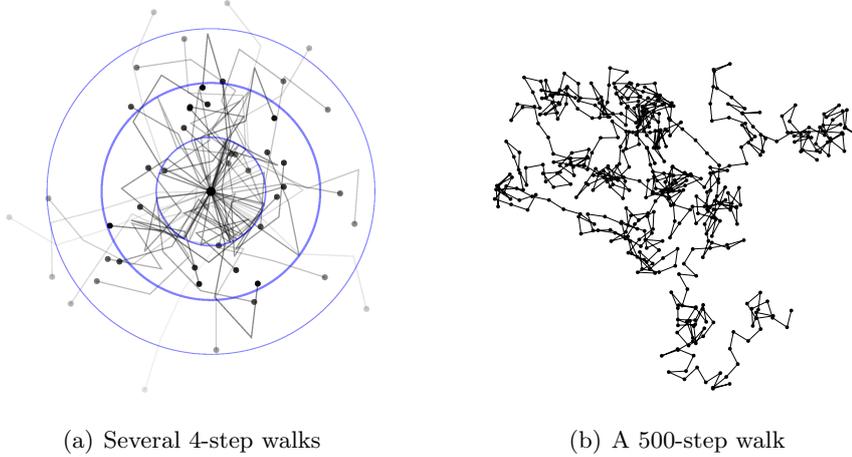


FIGURE 1. Random walks in the plane.

A related second motivation for our work is of numerical nature. In fact, more than 70 years after the problem was posed, [148] 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 (1.30) which is highly oscillatory, to reasonably high precision (see [177] for a general scheme). Some comments on obtaining high precision numerical evaluations of $W_n(s)$ are given in Appendix 1.6. A more comprehensive study of the numerics of such multiple-integrations is conducted in [19].

A lot is known about the one-dimensional random walk, the most basic random walk. It is a rather standard exercise in counting that the probability density for the n -step walk is $2^{-n} \binom{n}{(d+n)/2}$, where d is the signed distance from the origin. When the bottom term in the binomial coefficient is not an integer, the coefficient is understood to be 0. From this, it is easy to work out that the average distance from the origin after n steps is $(n-1)!!/(n-2)!!$ for n even and $n!!/(n-1)!!$ for n odd; and the second moment of the distance is n . (Here $n!! = n \cdot (n-2) \cdot (n-4) \cdots$ is the double factorial.) Asymptotically the average distance behaves like $\sqrt{2n/\pi}$.

For the two-dimensional walk no such explicit expressions were known, though the expected value for the root-mean-square distance is known to be \sqrt{n} ; in this case the implicit square root in (1.1) disappears which greatly simplifies the problem.

The term “random walk” first appears in a question by Karl Pearson in *Nature* in 1905 [159]. He asked for the probability density of a two-dimensional random walk expressed in the language of how far a “rambler” might walk. This triggered a response by Lord Rayleigh [165] 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 , x being the radial distance. This quickly leads to a good approximation for $W_n(s)$ for large n and fixed $s = 1, 2, 3, \dots$

Another week later, Pearson again wrote in *Nature*, see [160], 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 :

$$p_3(x) = \frac{\sqrt{x}}{\pi^2} \operatorname{Re} K\left(\sqrt{\frac{(x+1)^3(3-x)}{16x}}\right), \quad (1.3)$$

see e.g. [118] or [158]; Chapter 4 produces an elementary derivation. 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 , for the densities p_3 , p_4 and p_5 have remarkable features of their own.

The results obtained here, as well as in a follow-up study in Chapter 2 ([56]), have been crucial in the discovery of a closed form for the density p_4 of the distance traveled in 4 steps. It should be noted that the progress we make rely on techniques, for instance analysis of Meijer G-functions and their relationship with generalised hypergeometric series, that were fully developed only much later in the 20th century.

We remark that much has been done in generalising the problem posed by Pearson. For instance, Kluiver [123] made an analysis of the cumulative distribution function of the distance traveled in the plane for various choices of step lengths. Other generalisations include allowing walks in three dimensions (where the analysis is actually simpler, see [195, §49] and Chapter 4), confining the walks to different kinds of lattices, or calculating whether and when the walker would return to the origin. A good source of these sorts of results is [118].

Applications of two-dimensional random walks are numerous and well-known; for instance, [118] mentions that they may be used to model the random migration of an organism possessing flagella; analysing the superposition of waves (e.g.,

n	$s = 2$	$s = 4$	$s = 6$	$s = 8$	$s = 10$	[180]
2	2	6	20	70	252	A000984
3	3	15	93	639	4653	A002893
4	4	28	256	2716	31504	A002895
5	5	45	545	7885	127905	A169714
6	6	66	996	18306	384156	A169715

TABLE 1. $W_n(s)$ at even integers.

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. $W_n(s)$ at odd integers.

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 (1.1) from the common room at the University of New South Wales. It had been written down by Peter Donovan as a generalisation of a discrete cryptographic problem [87]. Some numerical values of W_n evaluated at integers are shown in Tables 1 and 2. One immediately notices the integrality of the sequences for the even moments, where the square root for $s = 2$ gives the root-mean-square distance. For $n = 2, 3, 4$ these sequences were found in the On-line Encyclopedia of Integer Sequences [180] – the cases $n = 5, 6$ are in the database as a consequence of this work.

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

$$W_3(k) = \operatorname{Re} {}_3F_2\left(\begin{matrix} \frac{1}{2}, -\frac{k}{2}, -\frac{k}{2} \\ 1, 1 \end{matrix} \middle| 4\right). \quad (1.4)$$

The evaluation (1.2) of $W_3(1)$ can be deduced from (1.4). Based on results in Sections 1.2 and 1.3, (1.4) is established in Section 1.5.

In Section 1.2 we prove 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 $f_n(k)$.

In Section 1.3 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. 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. Inspired by a general combinatorial convolution given in Section 1.2, we conjecture (1.28), which will be partially resolved in Chapter 3.

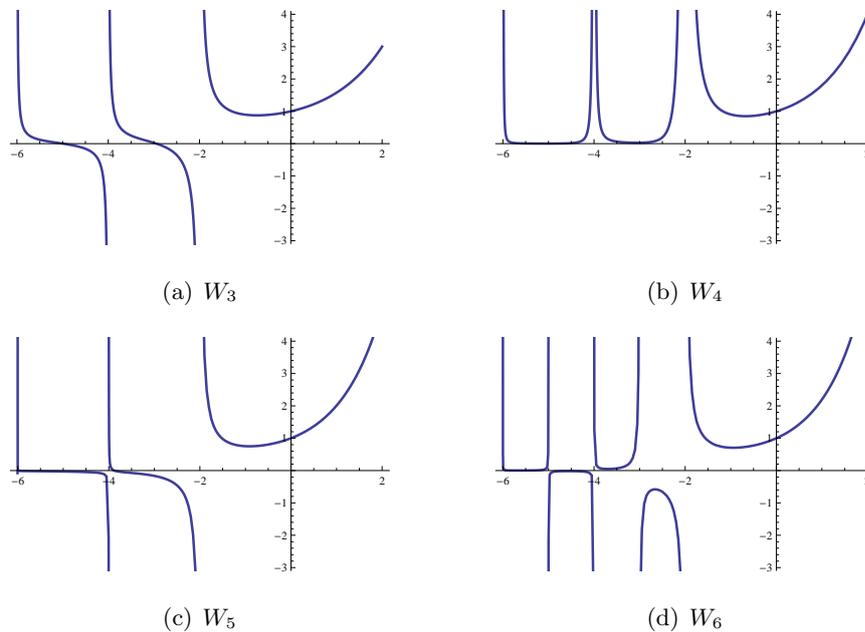


FIGURE 2. Various W_n and their analytic continuations.

1.2. The even moments and their combinatorial features

In the case $s = 2k$ the square root implicit in the definition (1.1) of $W_n(s)$ disappears, resulting in the fact that the even moments $W_n(2k)$ are integers. In this section we gather several of the combinatorial features of these moments which 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 1.5; the recurrence equation for $W_4(2k)$ is at the heart of the derivation of the closed form p_4 in Chapter 3 ([57]).

In fact, the even moments are given as sums of squares of multinomials – as is detailed next. While this result may also be obtained from probabilistic principles starting with the observation that the characteristic function of the distance traveled in n steps is J_0^n , we prefer to give an elementary derivation starting from the definition (1.1) of $W_n(s)$.

Proposition 1.1. *For nonnegative integers k and n ,*

$$W_n(2k) = \sum_{a_1+\dots+a_n=k} \binom{k}{a_1, \dots, a_n}^2. \quad (1.5)$$

PROOF. From the residue theorem of complex analysis, if $f(x_1, \dots, x_n)$ has a Laurent expansion around the origin then

$$\text{ct } f(x_1, \dots, x_n) = \int_{[0,1]^n} f(e^{2\pi i x_1}, \dots, e^{2\pi i x_n}) \, d\mathbf{x}, \quad (1.6)$$

where ‘ct’ extracts the constant term. In light of (1.6), (1.1) may be restated as

$$W_n(s) = \text{ct} \left((x_1 + \dots + x_n)(1/x_1 + \dots + 1/x_n) \right)^{s/2}. \quad (1.7)$$

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

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

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

Remark 1.2.1. In the case that s is not an even integer, the right-hand side of (1.7) may still be expanded, say, when $\text{Re } s \geq 0$ to obtain the series evaluation

$$W_n(s) = n^s \sum_{m \geq 0} (-1)^m \binom{s/2}{m} \sum_{k=0}^m \frac{(-1)^k}{n^{2k}} \binom{m}{k} \sum_{a_1+\dots+a_n=k} \binom{k}{a_1, \dots, a_n}^2. \quad (1.8)$$

In the spirit of experimental mathematics, we briefly outline the genesis of the evaluation given in Proposition 1.1.

In our first proof of the proposition, we showed that

$$\left| \sum_k e^{2\pi x_k i} \right|^2 = n^2 - 4 \sum_{i < j} \sin^2(\pi(x_j - x_i)),$$

and therefore, via binomial expansion, we have

$$W_n(s) = n^s \sum_{m \geq 0} \frac{(-1)^m}{n^{2m}} \binom{s/2}{m} \int_{[0,1]^n} \left(4 \sum_{i < j} \sin^2(\pi(x_j - x_i)) \right)^m d\mathbf{x}. \quad (1.9)$$

Let $I_{n,m}$ be defined by the multiple integral above. The sequence $2^{2m}I_{3,m}$ is Sloane's A093388 [180] where a link to [188] is given. That paper mentions that $2^{2m}I_{3,m}$ is 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 $(4xy - (x+y)(y+x))^m$. We then noticed that

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

and this line of extrapolation led to the correct form, i. e. the next case would involve $4^2wxyz - (w+x+y+z)(wxy+xyz+yzw+zxw)$. We thus conjectured that $2^{2m}I_{n,m}$ is the constant term of

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

which was proven by expanding the integrand in $I_{n,m}$ and invoking some combinatorial features of the expansion. This leads to (1.8), from which we may recover (1.5) for even s , using the binomial transform (see (11.12)). \diamond

In light of Proposition 1.1, we consider the combinatorial sums

$$f_n(k) = \sum_{a_1 + \cdots + a_n = k} \binom{k}{a_1, \dots, a_n}^2. \quad (1.10)$$

These numbers also appear in [166] 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). Given this enumerative interpretation, it is not hard to see that

$$f_{n_1+n_2}(k) = \sum_{j=0}^k \binom{k}{j}^2 f_{n_1}(j) f_{n_2}(k-j), \quad (1.11)$$

for two non-overlapping alphabets with n_1 and n_2 letters. In particular, we may use (1.11) to obtain $f_1(k) = 1$, $f_2(k) = \binom{2k}{k}$, as well as

$$f_3(k) = \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j} = {}_3F_2 \left(\begin{matrix} \frac{1}{2}, -k, -k \\ 1, 1 \end{matrix} \middle| 4 \right) = \binom{2k}{k} {}_3F_2 \left(\begin{matrix} -k, -k, -k \\ 1, -k + \frac{1}{2} \end{matrix} \middle| \frac{1}{4} \right), \quad (1.12)$$

$$f_4(k) = \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j} \binom{2(k-j)}{k-j} = \binom{2k}{k} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, -k, -k, -k \\ 1, 1, -k + \frac{1}{2} \end{matrix} \middle| 1 \right). \quad (1.13)$$

Here and below ${}_pF_q$ denotes the generalised hypergeometric function. In general, (1.11) can be used to write f_n as a sum with at most $\lceil n/2 \rceil - 1$ summation indices.

We remark that a generating function for $(f_n(k))_{k=0}^\infty$ is used in [20]. Let $I_n(z)$ denote the *modified Bessel function* of the first kind. Then

$$\sum_{k \geq 0} f_n(k) \frac{z^k}{k!^2} = \left(\sum_{k \geq 0} \frac{z^k}{k!^2} \right)^n = {}_0F_1(1; z)^n = I_0(2\sqrt{z})^n. \quad (1.14)$$

It can be anticipated from (1.10) 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 [29]; that paper gives the recursions for $3 \leq n \leq 6$ explicitly. An explicit general formula for the recurrences is given in [189]:

Theorem 1.1. *For fixed $n \geq 2$, the sequence $f_n(k)$ satisfies a recurrence of order $\lambda = \lceil n/2 \rceil$ with polynomial coefficients of degree $n - 1$:*

$$\sum_{j \geq 0} \left[k^{n-1} \sum_{\alpha_1, \dots, \alpha_j} \prod_{i=1}^j (-\alpha_i)(n+1-\alpha_i) \left(\frac{k-i}{k-i+1} \right)^{\alpha_i-1} \right] f_n(k-j) = 0. \quad (1.15)$$

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

The recursions for $n = 2, 3, 4, 5$ are listed in Example 1.3.2, formulated in terms of $W_n(s)$ as per Theorem 1.4. As a consequence of Theorem 1.1, we obtain:

Theorem 1.2. *For fixed $n \geq 2$, the sequence $f_n(k)$ satisfies a recurrence of order $\lambda = \lceil n/2 \rceil$ with polynomial coefficients of degree $n - 1$:*

$$c_{n,0}(k)f_n(k) + \dots + c_{n,\lambda}(k)f_n(k+\lambda) = 0 \quad (1.16)$$

$$\text{where } c_{n,0}(k) = (-1)^\lambda n!^2 \left(k + \frac{n}{4} \right)^{n+1-2\lambda} \prod_{j=1}^{\lambda-1} (k+j)^2, \quad (1.17)$$

and $c_{n,\lambda}(k) = (k+\lambda)^{n-1}$.

PROOF. The claim for $c_{n,\lambda}$ follows straight from (1.15). By (1.15), $c_{n,0}$ is given by

$$c_{n,0}(k-\lambda) = \left[k^{n-1} \sum_{\alpha_1, \dots, \alpha_\lambda} \prod_{i=1}^{\lambda} (-\alpha_i)(n+1-\alpha_i) \left(\frac{k-i}{k-i+1} \right)^{\alpha_i-1} \right] \quad (1.18)$$

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

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

$$c_{n,0}(k-\lambda) = (-1)^\lambda n!!^2 \prod_{j=1}^{\lambda-1} (k-j)^2 \quad (1.19)$$

in accordance with (1.17).

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

Now by (1.18), we have

$$c_{n,0}(k-\lambda) = (-1)^\lambda \left(\prod_{i=1}^{\lambda-1} (k-i)^2 \right) \sum_{j=0}^{\lambda} \left(\prod_{i=1}^{\lambda} a_i^j (n+1-a_i^j) \right) (k-\lambda+j), \quad (1.20)$$

where a_i^j denotes the i th element of a^j .

The sum in (1.20) has some symmetry, so writing it backwards and adding that to itself, we factor out the term involving k :

$$2 \sum_{j=0}^{\lambda} \left(\prod_{i=1}^{\lambda} a_i^j (n+1-a_i^j) \right) (k-\lambda+j) = (2k-\lambda) \sum_{j=0}^{\lambda} \prod_{i=1}^{\lambda} a_i^j (n+1-a_i^j). \quad (1.21)$$

As we know the sequences a^j explicitly, the product on the right of (1.21) 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 (1.21) is

$$\sum_{j=0}^{\lambda} (2\lambda)! \frac{\binom{2j}{j} \binom{2\lambda-2j}{\lambda-j}}{\binom{2\lambda}{\lambda}} = 2^{2\lambda} \lambda!^2, \quad (1.22)$$

which can be verified, for instance, using the snake oil method [197]. Substituting this into (1.20) gives (1.17) for even n . \square

Remark 1.2.2. 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

$$f_n(k) = \sum_{j=0}^k \binom{n}{j} \sum_{\substack{a_1+\dots+a_j=k \\ a_i>0}} \binom{k}{a_1, \dots, a_j}^2, \quad (1.23)$$

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

From (1.23) 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 [123]. In particular, $W_n(1) \approx_n \sqrt{n\pi}/2$. (This says that the sum of n random unit vectors in the plane has length around the order of \sqrt{n} .)

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

$$W_n(s) \approx_n n^{s/2-1} \left\{ \left(n - \frac{1}{2}\right) \Gamma\left(\frac{s}{2} + 1\right) + \Gamma\left(\frac{s}{2} + 2\right) - \frac{1}{4} \Gamma\left(\frac{s}{2} + 3\right) \right\}, \quad (1.24)$$

which is exact for $s = 0, 2, 4$; it is even indicative of the pole at $s = -2$ (see below). In particular, $W_n(1) \approx_n \sqrt{n\pi}/2 + \sqrt{\pi/n}/32$. More general approximations are given in [81]. \diamond

Remark 1.2.3. It follows straight from (1.10) that, for primes p , $f_n(p) \equiv n$ modulo p . Further, for $k \geq 1$, $f_n(k) \equiv n \pmod{2}$. This may be derived inductively from the recurrence (1.11) since, assuming that $f_n(k) \equiv n \pmod{2}$ for some n and all $k \geq 1$,

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

Hence for odd primes p ,

$$f_n(p) \equiv n \pmod{2p}. \quad (1.25)$$

The congruence (1.25) also holds for $p = 2$ since $f_n(2) = (2n - 1)n$ – compare with (1.23). In particular, (1.25) confirms that the last digit in the column for $s = 10$ is always $n \pmod{10}$ – an observation from Table 1. \diamond

Remark 1.2.4. The integers $f_3(k)$ (respectively $f_4(k)$) also arise in physics, see for instance [20], and are referred to as *hexagonal* (respectively *diamond*) *lattice integers*. The corresponding entries in Sloane's online encyclopedia [180] are A002893 and A002895. Both $f_3(k)$ and $f_4(k)$ are also Apéry-like sequences; see Chapter 11. We recall the following formulas [20, (186)–(188)], relating these sequences in non-obvious ways:

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

We are unable to find similar formulas connecting $f_5(k)$. \diamond

1.3. 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 $W_n(2k)$ extend to functional equations. This is deduced in the usual way from *Carlson's theorem*. We give the details, since the explicit form of the functional equations and the resulting pole structures are crucial for the discovery and proof of the closed forms in the cases $n = 3, 4, 5$ obtained in here and in Chapter 2 and 3.

1.3.1. 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.

Proposition 1.2. $W_n(s)$ is analytic at least for $\operatorname{Re} s > 0$.

PROOF. Let s_0 be a real number such that the integral in (1.1) 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 $s_0 < \operatorname{Re} s \leq s_0 + \lambda$ for some real $\lambda > 0$. For any real $0 \leq a \leq n$,

$$|a^s| = a^{\operatorname{Re} s} \leq n^\lambda a^{s_0},$$

and therefore

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

This local boundedness implies (see for instance [145]) that $W_n(s)$ as defined by the integral in (1.1) is analytic in s for $\operatorname{Re} s > s_0$. Since the integral clearly converges for $s = 0$, the claim follows. \square

This result will be extended in Theorem 1.5 and Corollary 1.1.

1.3.2. $n = 1$ and $n = 2$. It follows straight from the integral definition, or from the physical interpretation of the problem, that $W_1(s) = 1$. In the case $n = 2$, direct integration of (1.39) below yields

$$W_2(s) = 2^{s+1} \int_0^{1/2} \cos(\pi t)^s dt = \binom{s}{s/2}, \quad (1.26)$$

which may also be obtained using (1.8). 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 naïvely in form of the defining (1.1) (or expanded as the square root of a sum of squares), each returning the symbolic answer 0.

1.3.3. Functional equations. We may lift the recursive structure of f_n , defined in Section 1.2, to W_n on appealing to Carlson's theorem [185]. We recall that a function f is of *exponential type* in a region if $|f(z)| \leq M e^{c|z|}$ for some constants M and c .

Theorem 1.3 (Carlson). *Let f be analytic in the right half-plane $\operatorname{Re} z \geq 0$ and of exponential type with the additional requirement that*

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

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

Example 1.3.1. One obvious function f for which $f(k) = 0$ for $k = 0, 1, 2, \dots$ is $f(z) = \sin(\pi z)$. Here Carlson's theorem *does not* apply because the growth constant on the imaginary axis is exactly π . \diamond

Theorem 1.4. *Given that $f_n(k)$ satisfies a recurrence*

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

with polynomial coefficients $c_{n,j}(k)$ (see Theorem 1.2), then $W_n(s)$ satisfies the corresponding functional equation

$$c_{n,0}(s/2)W_n(s) + \cdots + c_{n,\lambda}(s/2)W_n(s + 2\lambda) = 0, \quad \text{for } \operatorname{Re} s \geq 0.$$

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 1.1, $U_n(s)$ 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 1.3 applies. By Proposition 1.2, $W_n(s)$ is analytic for $\operatorname{Re} s \geq 0$, and clearly $|W_n(s)| \leq n^{\operatorname{Re} s}$. Thus

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

In particular, $U_n(s)$ is of exponential type. Further, $U_n(s)$ is polynomially bounded on the imaginary axis $\operatorname{Re} s = 0$. Thus U_n satisfies the growth conditions of Carlson's Theorem. \square

Example 1.3.2. For $n = 2, 3, 4, 5$ we find

$$\begin{aligned} (s+2)W_2(s+2) - 4(s+1)W_2(s) &= 0, \\ (s+4)^2W_3(s+4) - 2(5s^2+30s+46)W_3(s+2) + 9(s+2)^2W_3(s) &= 0, \\ (s+4)^3W_4(s+4) - 4(s+3)(5s^2+30s+48)W_4(s+2) + 64(s+2)^3W_4(s) &= 0, \\ (s+6)^4W_5(s+6) - (35(s+5)^4 + 42(s+5)^2 + 3)W_5(s+4) + \\ (s+4)^2(259(s+4)^2 + 104)W_5(s+2) - 225(s+4)^2(s+2)^2W_5(s) &= 0. \end{aligned}$$

\diamond

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 $n \geq 3$. The case $n = 2$ is transparent, since $W_2(s) = \binom{s}{s/2}$ which has simple poles at the negative odd integers.

Theorem 1.5. *Let an integer $n \geq 3$ be given. The recursion guaranteed by Theorem 1.4 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 1.2 proves analyticity in the right half-plane. It is clear that the recursion given by Theorem 1.4 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

$$W_n(s) = -\frac{c_{n,1}(s/2)W_n(s+2) + \cdots + c_{n,\lambda}(s/2)W_n(s+2\lambda)}{c_{n,0}(s/2)} \quad (1.27)$$

with the $c_{n,j}$ as in (1.16). We observe that the right side of (1.27) only involves $W_n(s+2k)$ for $k \geq 1$. Therefore the least negative pole can only occur at a zero of $c_{n,0}(s/2)$ which is explicitly given in (1.17). We then note that the recursion forces poles to be simple or of order two, and to be replicated as claimed. \square

Corollary 1.1. *If $n \geq 3$ then $W_n(s)$, as given by (1.1), is analytic for $\operatorname{Re} s > -2$.*

PROOF. This follows directly from Theorem 1.5, the fact that $c_{n,0}(s/2)$ given in (1.17) has no zero for $s = -1$, and the proof of Proposition 1.2. \square

Example 1.3.3. In Figure 2, the analytic continuations for each of W_3 , W_4 , W_5 , and W_6 are plotted. Using the recurrence given in Example 1.3.2, we find that $W_3(s)$ has simple poles at $s = -2, -4, -6, \dots$. Similarly, we find that W_4 has double poles at $-2, -4, -6, \dots$ \diamond

Remark 1.3.1. More generally, it would appear that Theorem 1.5 can be extended to show that

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

This conjecture is further investigated in Chapter 2.

Knowledge about the poles of W_n for instance reveals the asymptotic behaviour of the probability densities at 0; this is detailed in Chapter 3. \diamond

1.3.4. Convolution series. Our attempt to lift the convolution sum (1.11) to $W_n(s)$ resulted in the following conjecture:

Conjecture 1.1. *For positive integers n and complex s ,*

$$W_{2n}(s) \stackrel{?}{=} \sum_{j \geq 0} \binom{s/2}{j}^2 W_{2n-1}(s-2j). \quad (1.28)$$

The right-hand side of (1.28) refers to the analytic continuation of W_n as guaranteed by Theorem 1.5. Conjecture 1.1, which is consistent with the pole structure described in Remark 1.3.1, has been confirmed by David Broadhurst [65] using a Bessel integral representation for W_n , given in (1.30), for $n = 2, 3, 4, 5$ and odd integers $s < 50$ to a precision of 50 digits. By (1.11) the conjecture clearly holds for s an even positive integer. For $n = 1$, we obtain from (1.28),

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

which agrees with (1.26).

A partial resolution of Conjecture 1.1 is one of our focuses; this is achieved in Chapter 3.

1.4. Bessel integral representations

As noted in the introduction, Kluyver [123] made a lovely analysis of the *cumulative distribution* function of the distance traveled for various fixed step lengths. In particular, for our uniform walk Kluyver provides the Bessel function representation

$$P_n(t) = t \int_0^\infty J_1(xt) J_0^n(x) dx. \quad (1.29)$$

Here and below $J_n(z)$ denotes the *Bessel function* of the first kind, defined by the series

$$J_n(z) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m! \Gamma(m+n+1)} \left(\frac{z}{2}\right)^{2m+n}.$$

Thus,

$$W_n(s) = \int_0^n t^s p_n(t) dt, \text{ where } p_n = P_n'.$$

From here, Broadhurst [65] obtains

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1 + \frac{s}{2})}{\Gamma(k - \frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x} \frac{d}{dx}\right)^k J_0^n(x) dx \quad (1.30)$$

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

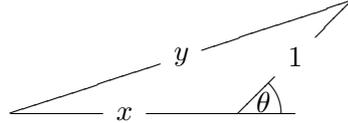
1.5. The odd moments of a three-step walk

In this section, we combine the results of the previous sections to finally prove the hypergeometric evaluation (1.4) of the moments $W_3(k)$ in Theorem 1.6.

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 exterior 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

$$g_s(x) := \frac{1}{\pi} \int_0^\pi y^s d\theta = |x + 1|^s {}_2F_1\left(\frac{1}{2}, -\frac{s}{2} \middle| \frac{4x}{(x + 1)^2}\right). \quad (1.31)$$

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

$$W_{n+1}(s) = \int_0^n g_s(x) p_n(x) dx, \quad (1.32)$$

where $p_n(x) = P'_n(x)$ 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 $p_2(x) = 2/(\pi\sqrt{4 - x^2})$ for $0 \leq x \leq 2$ and 0 otherwise. The density $p_3(x)$ is given in (1.3). More details for 2- and 3-step walks are given in Chapter 4.

For $n = 3$, based on (1.12) we define

$$V_3(s) := {}_3F_2\left(\frac{1}{2}, -\frac{s}{2}, -\frac{s}{2} \middle| 1, 1 \middle| 4\right), \quad (1.33)$$

so that by Proposition 1.1, $W_3(2k) = V_3(2k)$ 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 1.6. *For nonnegative even integers and all odd integers k :*

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

Remark 1.5.1. Note that, for all complex s , the function $V_3(s)$ also satisfies the recursion given in Example 1.3.2 for $W_3(s)$ – as is routine to prove using creative

telescoping [161]. However, V_3 does not satisfy the growth conditions of Carlson's Theorem 1.3. Thus, it yields another illustration that the hypotheses can fail. \diamond

PROOF OF THEOREM 1.6. It remains to prove the result for odd integers. Since, as noted in Remark 1.5.1, for all complex s , the function $V_3(s)$ also satisfies the recursion given in Example 1.3.2, it suffices to show that the values given for $s = 1$ and $s = -1$ are correct. From (1.32), we have the following expression:

$$W_3(s) = \frac{2}{\pi} \int_0^2 \frac{g_s(x)}{\sqrt{4-x^2}} dx = \frac{2}{\pi} \int_0^{\pi/2} g_s(2 \sin(t)) dt. \quad (1.34)$$

For $s = 1$: combining equation (1.31), [46, Exercise 1c], and Jacobi's imaginary transformations [46, Exercises 7a & 8b], we have

$$\frac{\pi}{2} g_1(x) = (x+1)E\left(\frac{2\sqrt{x}}{x+1}\right) = \operatorname{Re}(2E(x) - (1-x^2)K(x)). \quad (1.35)$$

Thus, from (1.34) and (1.35), and using the integral definitions of the complete elliptic integrals E and K ,

$$\begin{aligned} W_3(1) &= \frac{4}{\pi^2} \operatorname{Re} \int_0^{\pi/2} \left(2E(2 \sin(t)) - (1-4 \sin^2(t))K(2 \sin(t)) \right) dt \\ &= \frac{4}{\pi^2} \operatorname{Re} \int_0^{\pi/2} \int_0^{\pi/2} 2\sqrt{1-4 \sin^2(t) \sin^2(r)} dt dr \\ &\quad - \frac{4}{\pi^2} \operatorname{Re} \int_0^{\pi/2} \int_0^{\pi/2} \frac{1-4 \sin^2(t)}{\sqrt{1-4 \sin^2(t) \sin^2(r)}} dt dr. \end{aligned}$$

Amalgamating the two last integrals and parameterising, we consider

$$Q(a) := \frac{4}{\pi^2} \int_0^{\pi/2} \int_0^{\pi/2} \frac{1+a^2 \sin^2(t) - 2a^2 \sin^2(t) \sin^2(r)}{\sqrt{1-a^2 \sin^2(t) \sin^2(r)}} dt dr. \quad (1.36)$$

We now use the binomial theorem to integrate (1.36) term-by-term for $|a| < 1$ and substitute

$$\frac{2}{\pi} \int_0^{\pi/2} \sin^{2m}(t) dt = (-1)^m \binom{-\frac{1}{2}}{m}$$

throughout. Evaluation of the consequent infinite sum produces

$$\begin{aligned} Q(a) &= \sum_{k \geq 0} (-1)^k \binom{-\frac{1}{2}}{k} \left[a^{2k} \binom{-\frac{1}{2}}{k}^2 - a^{2k+2} \binom{-\frac{1}{2}}{k} \binom{-\frac{1}{2}}{k+1} - 2a^{2k+2} \binom{-\frac{1}{2}}{k+1}^2 \right] \\ &= \sum_{k \geq 0} (-1)^k a^{2k} \binom{-\frac{1}{2}}{k}^3 \frac{1}{(1-2k)^2} = {}_3F_2 \left(\begin{matrix} -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| a^2 \right). \end{aligned}$$

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

For $s = -1$: we similarly and more easily use (1.31) and (1.34) to derive

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

The corresponding imaginary transformation is $\frac{1}{x+1} K\left(\frac{2\sqrt{x}}{1+x}\right) = \operatorname{Re} K(x)$. \square

Example 1.5.1. Theorem 1.6 allows us to establish the following equivalent expressions for $W_3(1)$:

$$\begin{aligned} W_3(1) &= \frac{4\sqrt{3}}{3} \left({}_3F_2\left(-\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \middle| \frac{1}{4}\right) - \frac{1}{\pi} \right) + \frac{\sqrt{3}}{24} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{1}{4}\right) \\ &= 2\sqrt{3} \frac{K^2(k_3)}{\pi^2} + \sqrt{3} \frac{1}{K^2(k_3)} \\ &= \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4} \frac{2^{2/3}}{\pi^4} \Gamma^6\left(\frac{2}{3}\right). \end{aligned} \quad (1.37)$$

These rely on using Legendre's relation, Orr-type theorems, and the evaluation of $K(k_3)$ where $k_3 = \frac{\sqrt{3}-1}{2\sqrt{2}}$ is the third singular value of K [46]. (We come back to these tools in Chapter 12.)

More simply but similarly, we have

$$W_3(-1) = 2\sqrt{3} \frac{K^2(k_3)}{\pi^2} = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right). \quad (1.38)$$

Using the recurrence presented in Example 1.3.2, it follows that similar expressions can be given for W_3 evaluated at odd integers; see also Section 3.7. \diamond

Remark 1.5.2. As with (1.37),

$$\operatorname{Im} V_3(1) = -\frac{1}{8} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{1}{4}\right), \quad \operatorname{Re} V_3(-3) = \frac{\sqrt{3}}{72} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{1}{4}\right).$$

From the expansion (1.8) and the closed form for $W_3(1)$, we are thus able to evaluate the following sums:

$$\begin{aligned} W_3(1) &= 3 \sum_{n=0}^{\infty} \binom{\frac{1}{2}}{n} \left(-\frac{8}{9}\right)^n \sum_{k=0}^n \binom{n}{k} \left(-\frac{1}{8}\right)^k \sum_{j=0}^k \binom{k}{j}^3 \\ &= 3 \sum_{n=0}^{\infty} (-1)^n \binom{\frac{1}{2}}{n} \sum_{k=0}^n \binom{n}{k} \left(-\frac{1}{9}\right)^k \sum_{j=0}^k \binom{k}{j}^2 \binom{2j}{j}. \end{aligned}$$

\diamond

1.5.1. Conclusion. The behaviour of these two-dimensional walks provides a fascinating blend of probabilistic, analytic, algebraic and combinatorial challenges. In the next three chapters, we will continue our analysis of these walks, with a particular focus on the four-step walk.

1.6. Appendix: Numerical evaluations

A one-dimensional reduction of the integral (1.1) may be achieved by taking symmetry into account:

$$W_n(s) = \int_{[0,1]^{n-1}} \left| 1 + \sum_{k=1}^{n-1} e^{2\pi i x_k} \right|^s d(x_1, \dots, x_{n-1}). \quad (1.39)$$

Note, though, that this form breaks the symmetry in the integrand and is not conducive for proofs, such as that of Proposition 1.1. For $n > 5$, it is very hard to evaluate high dimensional integrals such as (1.39) to any reasonable precision using schemes like Gaussian or tanh-sinh quadrature [23].

From (1.39), 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 [79] 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 (1.30) seems very good for high precision evaluations of $W_n(s)$. We close by commenting on the special cases $n = 3, 4$.

Example 1.6.1. The first high precision evaluations of W_3 were performed by David Bailey who confirmed Theorem 1.6 for $s = 2, \dots, 7$ to 175 digits. This was done on a 256-core LBNL system in roughly 15 minutes by applying tanh-sinh integration to

$$W_3(s) = \int_0^1 \int_0^1 (9 - 4(\sin^2(\pi x) + \sin^2(\pi y) + \sin^2(\pi(x - y))))^{s/2} dy dx,$$

which is obtained from (1.39). More practical is the one-dimensional form (1.34) which can deliver high precision results in minutes on a laptop. For integral s , Theorem 1.6 allows extremely high precision evaluations. \diamond

Example 1.6.2. Assuming that Conjecture 1.1 holds for $n = 2$ (for a proof, see Chapter 3), Theorem 1.6 implies that for nonnegative integers k

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

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. \diamond

CHAPTER 2

Three-Step and Four-Step Random Walk Integrals

ABSTRACT. We investigate the moments of distances of 3- and 4-step uniform random walks in the plane. We further analyse a formula conjectured in Chapter 1 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.

2.1. Introduction and preliminaries

Continuing research commenced in [53] (Chapter 1), for complex s , we consider the n -dimensional integral

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

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. As such, the integral (2.1) expresses the s th moment of the distance to the origin after n steps. The study of such walks provides interesting numeric and symbolic computation challenges; indeed, nearly all of our results were discovered *experimentally*.

We recall that for $n \geq 3$, the integral (2.1) is well-defined and analytic for $\operatorname{Re} s > -2$, and admits an analytic continuation to the complex plane with poles at certain negative integers.

For s an even positive integer, we have

$$W_n(2k) = \sum_{a_1 + \dots + a_n = k} \binom{k}{a_1, \dots, a_n}^2. \quad (2.2)$$

Furthermore, as proved in Chapter 1, we have

$$W_3(1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right) + \frac{27}{4} \frac{2^{2/3}}{\pi^4} \Gamma^6\left(\frac{2}{3}\right), \quad (2.3)$$

$$W_3(-1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6\left(\frac{1}{3}\right). \quad (2.4)$$

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

2.2. Bessel integral representations

We start with the result of Kluyver [123], amplified in [195, §31.48] and exploited in Chapter 1, to the effect that the probability that an n -step walk ends up within a disc of radius α is

$$P_n(\alpha) = \alpha \int_0^\infty J_1(\alpha x) J_0^n(x) dx. \quad (2.5)$$

From this, Broadhurst [65] obtains

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1 + \frac{s}{2})}{\Gamma(k - \frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x} \frac{d}{dx} \right)^k J_0^n(x) dx \quad (2.6)$$

valid as long as $2k > s > -n/2$.

Example 2.2.1 ($W_n(\pm 1)$). In particular, from (2.6), for $n > 2$, we can write:

$$W_n(-1) = \int_0^\infty J_0^n(x) dx, \quad W_n(1) = n \int_0^\infty J_1(x) J_0(x)^{n-1} \frac{dx}{x}. \quad (2.7)$$

For $0 < s < n/2$, we have

$$W_n(-s) = 2^{1-s} \frac{\Gamma(1 - s/2)}{\Gamma(s/2)} \int_0^\infty x^{s-1} J_0^n(x) dx, \quad (2.8)$$

so that $W_n(-s)$ essentially is the analytic continuation of the *Mellin transform* (see e. g. [118]) of the n th power of the Bessel function J_0 . \diamond

Example 2.2.2. Using (2.8), the fact that $W_1(s) = 1$ and $W_2(s) = \binom{s}{s/2}$ translates into the evaluations

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

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 2.2 and 2.3. \diamond

Remark 2.2.1. Here, we demonstrate how Ramanujan’s ‘master theorem’ may be applied to find the Bessel integral representation (2.6) in a natural way.

Ramanujan’s master theorem [112, 9] states that, under certain conditions on the analytic function φ ,

$$\int_0^\infty x^{\nu-1} \left(\sum_{k=0}^\infty \frac{(-x)^k}{k!} \varphi(k) \right) dx = \Gamma(\nu) \varphi(-\nu). \quad (2.9)$$

The proof is based on the residue theorem and the inverse Mellin transform.

Based on the evaluation (2.2), we have, as noted in Chapter 1, the generating function

$$\sum_{k \geq 0} W_n(2k) \frac{(-x)^k}{(k!)^2} = \left(\sum_{k \geq 0} \frac{(-x)^k}{(k!)^2} \right)^n = J_0(2\sqrt{x})^n \quad (2.10)$$

for the even moments. Applying Ramanujan’s master theorem (2.9) to $\varphi(k) := W_n(2k)/k!$, we find

$$\Gamma(\nu) \varphi(-\nu) = \int_0^\infty x^{\nu-1} J_0^n(2\sqrt{x}) dx. \quad (2.11)$$

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

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

This is the case $k = 0$ of (2.6). 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 $(-\frac{1}{x} \frac{d}{dx})^k f(x)$. \diamond

2.2.1. Pole structure. A very useful consequence of equation (2.8) is the following proposition.

Proposition 2.1 (Poles). *The structure of the poles of W_n is as follows:*

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

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

and the corresponding poles are simple.

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

$$\text{Res}_{(-2k-2)}(W_n) = \frac{(-1)^k}{4^k k!^2} \int_0^\infty x^{2k+1} J_0^n(x) dx. \quad (2.12)$$

(c) Moreover, for odd $n \geq 5$, 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 2.1. For individual n this may be verified as in Example 2.2.3. This was done by the authors for $n \leq 45$.

PROOF. (a) $\text{Res}_{-2}(W_3) = 2/(\sqrt{3}\pi)$ from [195, p. 412], since it is the value of $\int_0^\infty xJ_0^3(x) dx$ in accordance with (2.12). Letting $r_3(k) := \text{Res}_{(-2k)}(W_n)$, the explicit residue equation is

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

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

$$(s+4)^2 W_3(s+4) - 2(5s^2 + 30s + 46)W_3(s+2) + 9(s+2)^2 W_3(s) = 0. \quad (2.13)$$

We give another derivation in Example 2.3.2.

(b) For $n \geq 5$ we note that the integral in (2.12) is absolutely convergent since $|J_0(x)| \leq 1$ on the real axis and $J_0(x) \approx \sqrt{2/(\pi x)} \cos(x - \pi/4)$, see [2, (9.2.1)]. Since

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

the residue is as claimed by (2.8).

(c) As shown in Chapter 1, 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 $\text{Res}_{(-2k)}(W_n)$ for $k = 1, 2, \dots$. 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 $4|n$.

□

Example 2.2.3 (Poles of W_5). We illustrate Proposition 2.1 in the case $n = 5$. We start with the recursion:

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

From here,

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

which shows that the first pole is indeed simple as is also guaranteed by Proposition 2.1b. Similarly,

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

showing that the second pole is simple as well. It follows from Proposition 2.1c that all poles of W_5 are simple. More specifically, let $r_5(k) := \text{Res}_{(-2k)}(W_5)$. With initial values $r_5(0) = 0, r_5(1)$ and $r_5(2)$, we derive that

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

◇

Example 2.2.4 (Poles of W_4). Let $r_4(k) := \lim_{s \rightarrow -2k} (s+2k)^2 W_4(s)$, then the recursion for $W_4(s)$

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

gives

$$r_4(k+2) = \frac{1}{32} \frac{(2k+1)(5k^2 + 5k + 2)}{(k+1)^3} r_4(k+1) - \frac{1}{64} \frac{k^3}{(k+1)^3} r_4(k).$$

We also compute that

$$\frac{3}{2\pi^2} = r_4(1) = \lim_{s \rightarrow -2} (s+2)^2 W_4(s) = \frac{3 + 4W_4'(0) - W_4'(2)}{8}.$$

The first equality is obtainable from (2.19) in the next chapter. Further, L'Hôpital's rule shows that the residue at $s = -2$ is

$$\lim_{s \rightarrow -2} \frac{d}{ds} ((s+2)^2 W_4(s)) = \frac{9 + 18W_4'(0) - 3W_4'(2) + 4W_4''(0) - W_4''(2)}{16}$$

with a numerical value of $0.316037\dots$ which we were able to identify as $\frac{9}{2\pi^2} \log(2)$. This is proven in Chapter 3, section 6.

We finally record a remarkable identity related to the pole of W_4 at -2 that was established in [195, p. 415]:

$$\int_0^\infty J_\nu^A(x) x^{1-2\nu} dx = \frac{1}{2\pi} \frac{\Gamma(2\nu)\Gamma(\nu)}{\Gamma(3\nu)\Gamma(\nu + 1/2)}.$$

◇

2.2.2. 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} [32], by

$$\begin{aligned} G_{p,q}^{m,n} \left(\begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \middle| x \right) &= G_{p,q}^{m,n} \left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix} \middle| x \right) \\ &= \frac{1}{2\pi i} \int_L \frac{\prod_{k=1}^m \Gamma(b_k - t) \prod_{k=1}^n \Gamma(1 - a_k + t)}{\prod_{k=m+1}^q \Gamma(1 - b_k + t) \prod_{k=n+1}^p \Gamma(a_k - t)} x^t dt. \end{aligned} \quad (2.14)$$

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 $G_{m,n}^{p,q}$ is analytic in each parameter, in consequence so are the compositions arising below.

Our main tool below is the following consequence of the Mellin convolution formula [118], giving the Mellin transform of a product.

Theorem 2.1. *Let $G(s)$ and $H(s)$ be the Mellin transforms of $g(x)$ and $h(x)$ respectively. Then*

$$\int_0^\infty x^{s-1} g(x) h(x) dx = \frac{1}{2\pi i} \int_{\delta-i\infty}^{\delta+i\infty} G(z) H(s-z) dz \quad (2.15)$$

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

This leads to:

Theorem 2.2 (Meijer form for W_3). *For all complex s*

$$W_3(s) = \frac{\Gamma(1+s/2)}{\sqrt{\pi}\Gamma(-s/2)} G_{3,3}^{2,1} \left(\begin{matrix} 1, 1, 1 \\ 1/2, -s/2, -s/2 \end{matrix} \middle| \frac{1}{4} \right). \quad (2.16)$$

PROOF. We apply Theorem 2.1 to $J_0^3 = J_0^2 \cdot J_0$ for s in a vertical strip. Using Example 2.2.2 we then obtain

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

where $0 < \delta < 1$. The claim follows from (2.8) by analytic continuation. \square

Similarly we obtain:

Theorem 2.3 (Meijer form for W_4). *For all complex s with $\operatorname{Re} s > -2$*

$$W_4(s) = \frac{2^s \Gamma(1 + s/2)}{\pi \Gamma(-s/2)} G_{4,4}^{2,2} \left(\begin{matrix} 1, (1 - s)/2, 1, 1 \\ 1/2, -s/2, -s/2, -s/2 \end{matrix} \middle| 1 \right). \quad (2.17)$$

PROOF. We now apply Theorem 2.1 to $J_0^4 = J_0^2 \cdot J_0^2$, again for s in a vertical strip. Using once more Example 2.2.2, we obtain

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

where $0 < \delta < 1$. The claim again follows from (2.8). \square

We illustrate with graphs of W_3, W_4 in the complex plane in Figure 1. 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 was employed for s with $\operatorname{Re} s \leq -2$.

2.2.3. Hypergeometric representations. Slater's theorem [142, p. 57] expands certain classes of Meijer G -functions in terms of hypergeometric functions. In particular, $W_3(s)$ and $W_4(s)$ as given in Theorems 2.2 and 2.3 can be expanded.

Corollary 2.1 (Hypergeometric forms). *For s not an odd integer, we have*

$$W_3(s) = \frac{\tan\left(\frac{\pi s}{2}\right)}{2^{2s+1}} \left(\frac{s}{2}\right)^2 {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{s+3}{2}, \frac{s+3}{2} \end{matrix} \middle| \frac{1}{4}\right) + \left(\frac{s}{2}\right) {}_3F_2\left(\begin{matrix} -\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \\ 1, -\frac{s-1}{2} \end{matrix} \middle| \frac{1}{4}\right), \quad (2.18)$$

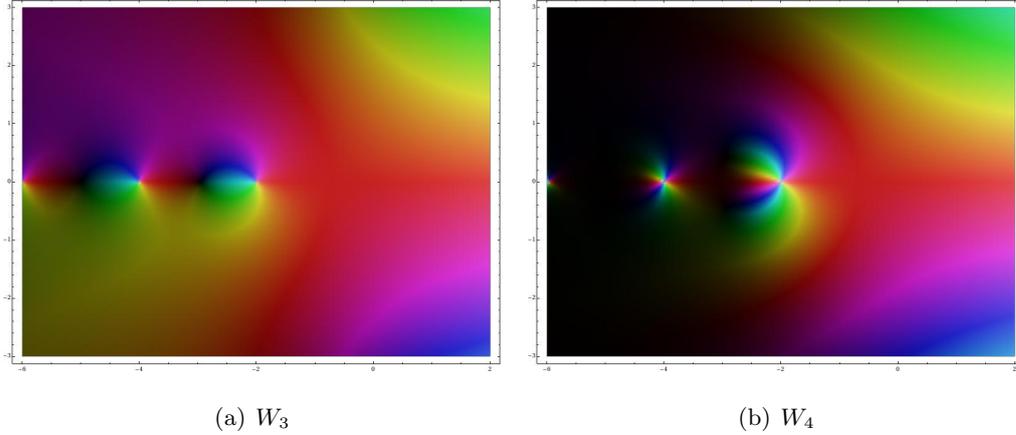


FIGURE 1. W_3 via (2.16) and W_4 via (2.17) in the complex plane.

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

$$W_4(s) = \frac{\tan\left(\frac{\pi s}{2}\right)}{2^{2s}} \binom{s}{\frac{s-1}{2}}^3 {}_4F_3\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{s}{2} + 1 \middle| \frac{s+3}{2}, \frac{s+3}{2}, \frac{s+3}{2} \middle| 1\right) + \binom{s}{\frac{s}{2}} {}_4F_3\left(\frac{1}{2}, -\frac{s}{2}, -\frac{s}{2}, -\frac{s}{2} \middle| 1, 1, -\frac{s-1}{2} \middle| 1\right). \quad (2.19)$$

These analytic continuations of W_3 and W_4 , first found in [81], can also be obtained by symbolic integration of (2.6) in *Mathematica*. We note that for $s = 2k = 0, 2, 4, \dots$ the first term in (2.18) (resp. (2.19)) is zero and the second is a formula given in (1.12) (resp. (1.13)). Thus, one can in principle also prove (2.18) and (2.19) by applying Carlson's theorem – after showing the singularities at $1, 3, 5, \dots$ are removable.

Example 2.2.5. From (2.18) and taking the limit using L'Hôpital's rule, we have

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

In conjunction with (2.4), we obtain the sum

$$\sum_{n=0}^{\infty} \binom{2n}{n}^3 \frac{\sum_{k=1}^{2n} \frac{(-1)^k}{k}}{4^{4n}} = \frac{\Gamma^6\left(\frac{1}{3}\right)(3\pi - 8\sqrt{3}\log 2)}{24 \cdot 2^{2/3}\pi^4}.$$

For comparison, (2.19) produces

$$W_4(-1) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4}{4^{4n}} \sum_{k=2n+1}^{\infty} \frac{(-1)^{k+1}}{k}. \quad (2.20)$$

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We see that while Corollary 2.1 makes it easy to analyse the poles, the removable singularities at the odd integers are much harder to resolve explicitly. For $W_4(-1)$ we proceed as follows:

Theorem 2.4 (Hypergeometric form for $W_4(-1)$).

$$W_4(-1) = \frac{\pi}{4} {}_7F_6 \left(\begin{matrix} \frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{1}{4}, 1, 1, 1, 1, 1 \end{matrix} \middle| 1 \right). \quad (2.21)$$

PROOF. Using Theorem 2.3 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 (2.14) of the Meijer G-function as a contour-integral, we see that the corresponding integrand is

$$\frac{\Gamma(\frac{1}{2} - t)^2 \Gamma(t)^2}{\Gamma(\frac{1}{2} + t)^2 \Gamma(1 - t)^2} x^t = \frac{\Gamma(\frac{1}{2} - t)^2 \Gamma(t)^4}{\Gamma(\frac{1}{2} + t)^2} \cdot \frac{\sin^2(\pi t)}{\pi^2} x^t, \quad (2.22)$$

where we have used the reflection formula $\Gamma(t)\Gamma(1 - t) = \pi/\sin(\pi t)$ [196]. 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. The right-hand side of (2.22) can then be identified with the integrand of another Meijer G-function; thus we have shown that

$$G_{4,4}^{2,2} \left(\begin{matrix} 1, 1, 1, 1 \\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \end{matrix} \middle| 1 \right) = \frac{1}{\pi^2} G_{4,4}^{2,4} \left(\begin{matrix} 1, 1, 1, 1 \\ \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \end{matrix} \middle| 1 \right). \quad (2.23)$$

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 [32]

$$x^\alpha G_{p,q}^{m,n} \left(\begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \middle| x \right) = G_{p,q}^{m,n} \left(\begin{matrix} \mathbf{a} + \alpha \\ \mathbf{b} + \alpha \end{matrix} \middle| x \right) \quad (2.24)$$

we deduce that

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

Finally, we appeal to Bailey's identity [24, (3.4)]:

$$\begin{aligned} & {}_7F_6 \left(\begin{matrix} a, 1 + \frac{a}{2}, b, c, d, e, f \\ \frac{a}{2}, 1 + a - b, 1 + a - c, 1 + a - d, 1 + a - e, 1 + a - f \end{matrix} \middle| 1 \right) \\ &= \frac{\Gamma(1 + a - b)\Gamma(1 + a - c)\Gamma(1 + a - d)\Gamma(1 + a - e)\Gamma(1 + a - f)}{\Gamma(1 + a)\Gamma(b)\Gamma(c)\Gamma(d)\Gamma(1 + a - b - c)\Gamma(1 + a - b - d)\Gamma(1 + a - c - d)\Gamma(1 + a - e - f)} \\ & \quad \times G_{4,4}^{2,4} \left(\begin{matrix} e + f - a, 1 - b, 1 - c, 1 - d \\ 0, 1 + a - b - c - d, e - a, f - a \end{matrix} \middle| 1 \right). \end{aligned} \quad (2.25)$$

The claim follows upon setting all parameters to $1/2$. \square

An attempt to analogously apply Bailey's identity for $W_4(1)$ fails, since its Meijer G representation as obtained from Theorem 2.3 does not meet the precise form required in the formula. Nevertheless, a combination of Nesterenko's theorem [153] and Zudilin's theorem [207] gives the following result:

Theorem 2.5 (Hypergeometric form for $W_4(1)$).

$$W_4(1) = \frac{3\pi}{4} {}_7F_6 \left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 1, 1 \end{matrix} \middle| 1 \right) - \frac{3\pi}{8} {}_7F_6 \left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 2, 1 \end{matrix} \middle| 1 \right). \quad (2.26)$$

PROOF. We first prove a result that will allow us to apply 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:

$$\frac{d}{dz} \left(z^{-b_1} G_{4,4}^{2,2} \left(\begin{matrix} a_1, a_2, a_3, a_4 \\ b_1, b_2, b_3, b_4 \end{matrix} \middle| z \right) \right) = -z^{-1-b_1} G_{4,4}^{2,2} \left(\begin{matrix} a_1, a_2, a_3, a_4 \\ b_1 + 1, b_2, b_3, b_4 \end{matrix} \middle| z \right), \quad (2.27)$$

$$\frac{d}{dz} \left(z^{1-a_1} G_{4,4}^{2,2} \left(\begin{matrix} a_1, a_2, a_3, a_4 \\ b_1, b_2, b_3, b_4 \end{matrix} \middle| z \right) \right) = z^{-a_1} G_{4,4}^{2,2} \left(\begin{matrix} a_1 - 1, a_2, a_3, a_4 \\ b_1, b_2, b_3, b_4 \end{matrix} \middle| z \right). \quad (2.28)$$

Let $a(z) := G_{4,4}^{2,2} \left(\begin{matrix} 0, 1, 1, 1 \\ -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \end{matrix} \middle| z \right)$. Note that $a(1) = -2\pi W_4(1)$ by Theorem 2.3. Applying (2.27) to $a(z)$ and using the product rule, we get $\frac{1}{2}a(1) + a'(1) = c_1$, where

$$c_1 := -G_{4,4}^{2,2} \left(\begin{matrix} 0, 1, 1, 1 \\ \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2} \end{matrix} \middle| 1 \right).$$

Applying (2.28) and (2.24) to $a(z)$, we obtain $a'(1) = b_1$ where

$$b_1 := G_{4,4}^{2,2} \left(\begin{matrix} -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 0, -1, -1, -1 \end{matrix} \middle| 1 \right).$$

Appealing to

$$G_{p,q}^{m,n} \left(\begin{matrix} \mathbf{a} \\ \mathbf{b} \end{matrix} \middle| x \right) = G_{q,p}^{n,m} \left(\begin{matrix} 1 - \mathbf{b} \\ 1 - \mathbf{a} \end{matrix} \middle| \frac{1}{x} \right), \quad (2.29)$$

we see that $b_1 = -c_1$. Hence $a(1) = 4c_1$. Converting c_1 to a $G_{4,4}^{2,4}$ as in (2.23), which finally satisfies the conditions of Nesterenko's theorem, we obtain:

$$W_4(1) = \frac{4}{\pi^3} \int_0^1 \int_0^1 \int_0^1 \sqrt{\frac{x(1-y)(1-z)}{(1-x)yz(1-x(1-yz))}} dx dy dz.$$

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 thus obtain the result as claimed. \square

Zudilin's theorem will again be used in Chapter 6, and a statement of the theorem can be found there. Armed with closed forms for $W_4(\pm 1)$, we may thus find $W_4(s)$ for positive integer s using the recursion. The following alternative relation was first predicted by the *integer relation algorithm* PSLQ [18] in a computational hunt for results similar to that in Theorem 2.4:

Theorem 2.6 (Alternative hypergeometric form for $W_4(1)$).

$$W_4(1) = \frac{9\pi}{4} {}_7F_6\left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 1, 1 \end{matrix} \middle| 1\right) - 2\pi {}_7F_6\left(\begin{matrix} \frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{1}{4}, 1, 1, 1, 1, 1 \end{matrix} \middle| 1\right). \quad (2.30)$$

PROOF. For notational convenience, let

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

By (2.26), $W_4(1) = (32/\pi^3)(A - B)$, and the truth of (2.30) 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

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

and can be reduced to a one dimensional integral:

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

Here, as usual, $K'(k) := K(\sqrt{1 - k^2})$ 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 ([208], remark after lemma 8). We obtain

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

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

$$B = B_2 := \int_0^1 k^2 K'(k)^2 dk.$$

But B also satisfies the conditions of Bailey's identity and Nesterenko's theorem [153], from which we are able to produce an alternative triple integral, and reduce it to:

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

As for C , equation (2.51) below details its evaluation, which we also record here:

$$C = \int_0^1 K'(k)^2 dk.$$

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

Note that the theorem gives the identity

$$2 \int_0^1 K'(k) E'(k) dk = \int_0^1 (1 - k^2) K'(k)^2 dk, \quad (2.31)$$

among others. Equivalently, an independent proof of this identity means the non-trivial action is not needed – this is done in Chapter 6.

Remark 2.2.2. Each of the ${}_7F_6$'s involved in Theorems 2.4, 2.5 and 2.6 can also be easily written as a sum of two ${}_6F_5$'s. In Chapter 6, we actually express $W_4(-1)$ as the sum of two ${}_4F_3$'s.

The first ${}_7F_6$ term in Theorem 2.6 satisfies the conditions of Bailey's identity (2.25) (with $a = e = f = \frac{3}{2}, b = c = d = \frac{1}{2}$):

$${}_7F_6 \left(\begin{matrix} \frac{7}{4}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{4}, 2, 2, 2, 1, 1 \end{matrix} \middle| 1 \right) = -\frac{16}{3\pi^4} G_{4,4}^{2,4} \left(\begin{matrix} \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 0, 0, 0 \end{matrix} \middle| 1 \right). \quad (2.32)$$

We can thence convert the right-hand side of (2.30) to a Meijer G form. On the other hand,

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

So we obtain the non-trivial identity:

$$G_{4,4}^{2,4} \left(\begin{matrix} \frac{1}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \\ 1, 0, 0, 0 \end{matrix} \middle| 1 \right) = 24 G_{4,4}^{2,4} \left(\begin{matrix} \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 0, 0, 0 \end{matrix} \middle| 1 \right) + 8 G_{4,4}^{2,4} \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 0, 0, 0, 0 \end{matrix} \middle| 1 \right). \quad (2.33)$$

\diamond

Corollary 2.2 (Elliptic integral representation for $W_4(1)$). *We have*

$$W_4(1) = \frac{16}{\pi^3} \int_0^1 (1 - 3k^2) K'(k)^2 dk. \quad (2.34)$$

PROOF. The conclusion of Theorem 2.6 implies $(\pi^3/16)W_4(1) = C - 3B = C - 3B_2$, and the corollary follows. \square

2.3. Probabilistically inspired representations

In this section, we build on the probabilistic approach taken in Chapter 1. We may profitably view a $(m+n)$ -step walk as a composition of an m -step and n -step walk for $m, n \geq 1$. 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. Following the analysis in Chapter 1 using the cosine rule, 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

$$g_s(x, y) := \frac{1}{\pi} \int_0^\pi z^s d\theta = |x - y|^s {}_2F_1\left(\frac{1}{2}, -\frac{s}{2} \middle| 1 - \frac{4xy}{(x-y)^2}\right). \quad (2.35)$$

Remark 2.3.1 (Alternate forms for g_s). Using Kummer's quadratic transformation [11], we obtain

$$g_s(x, y) = \operatorname{Re} y^s {}_2F_1\left(-\frac{s}{2}, -\frac{s}{2} \middle| \frac{x^2}{y^2}\right) \quad (2.36)$$

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

$$\begin{aligned} g_{-1}(x, y) &= \operatorname{Re} \frac{2}{\pi y} K\left(\frac{x}{y}\right), \\ g_1(x, y) &= \operatorname{Re} \frac{2y}{\pi} \left\{ 2E\left(\frac{x}{y}\right) - \left(1 - \frac{x^2}{y^2}\right) K\left(\frac{x}{y}\right) \right\}. \end{aligned}$$

This second equation has various re-expressions. \diamond

Denote by $p_n(x)$ the probability 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

$$W_{n+m}(s) = \int_0^n \int_0^m g_s(x, y) p_n(x) p_m(y) dy dx, \quad (2.37)$$

for $s \geq 0$. Since for the 1-step walk we have $p_1(x) = \delta_1(x)$, this generalises the corresponding formula given for $W_{n+1}(s)$ in equation (1.32).

In (2.37), if $n = 0$, then we may take $p_0(x) = \delta_0(x)$, and regard the limits of integration as from $-\epsilon$ and $+\epsilon$, $\epsilon \rightarrow 0$. Then $g_s = y^s$ as the hypergeometric function

collapses to 1, and we recover the basic form

$$W_m(s) = \int_0^m y^s p_m(y) dy. \quad (2.38)$$

Remark 2.3.2. We can use the sine rule to make a change variable, changing the dy integral in (2.37) into dz , where $y = \sqrt{x^2 + z^2 - 2xz \cos t}$:

$$W_{n+m}(s) = \int_0^{n+m} z^s \left\{ \int_0^n \int_0^\pi \frac{z}{\pi y} p_n(x) p_m(y) dt dx \right\} dz. \quad (2.39)$$

By uniqueness of the density, the expression inside the braces is p_{n+m} . As one consequence, we obtain a numerically workable expression,

$$p_4(\alpha) = \frac{8\alpha}{\pi^3} \int_0^2 \operatorname{Re} \frac{K\left(\sqrt{\frac{16x\alpha}{(x+\alpha)^2(4-(x-\alpha)^2)}}\right)}{(x+\alpha)\sqrt{4-(x-\alpha)^2}} \frac{dx}{\sqrt{4-x^2}}. \quad (2.40)$$

◇

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

$$p_3(x) = \operatorname{Re} \frac{\sqrt{x}}{\pi^2} K\left(\sqrt{\frac{(x+1)^3(3-x)}{16x}}\right), \quad (2.41)$$

using p_2 and (2.39). To make (2.41) more accessible we can use the following cubic identity.

Proposition 2.2. *For all $0 \leq x \leq 1$ 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. The proof is typical of the ‘automatic’ approached championed in experimental mathematics. 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. Note that this is actually a re-parametrisation of the degree 3 modular equation (10.22). □

We apply Jacobi’s imaginary transform [46, p. 73], $\operatorname{Re} K(x) = \frac{1}{x} K\left(\frac{1}{x}\right)$ for $x > 1$, to express $p_3(x)$ as a real function over $[0, 1]$ and $[1, 3]$, leading to

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

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

$$W_3(-1) = 2 \int_0^1 \frac{p_3(x)}{x} dx. \quad (2.42)$$

To make sense of this observation more abstractly, let

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

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

$$p_3(x) = \frac{4x}{(3-x)(x+1)} p_3(\sigma(x)). \quad (2.43)$$

Example 2.3.1 (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 (2.2)). Using Proposition 2.2, we may now apply equation (184) in [20, Section 5.10] to obtain

$$p_3(x) = \frac{2x}{\pi\sqrt{3}} \sum_{k=0}^{\infty} W_3(2k) \left(\frac{x}{3}\right)^{2k}, \quad (2.44)$$

with radius of convergence 1. For $1 < x < 3$, on using (2.43) we obtain

$$p_3(x) = \frac{8x}{\pi\sqrt{3}(x+1)^2} \sum_{k=0}^{\infty} W_3(2k) \left(\frac{3-x}{3+3x}\right)^{2k}. \quad (2.45)$$

From (2.44) and (2.42) we deduce

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

compare with (2.56). ◇

Example 2.3.2 (Poles of W_3). From here we may efficiently recover the explicit form for the residues of W_3 given in Proposition 2.1a. Fix integers $N > 2k > 0$ and $0 < \alpha < 1$. Use the series $p_3(x) = \sum_{j \geq 0} a_j x^{2j+1}$ in (2.44) to write

$$\begin{aligned} W_3(s) - \int_{\alpha}^3 p_3(x) x^s dx - \int_0^{\alpha} \sum_{j=N}^{\infty} a_j x^{2j+1+s} dx &= \int_0^{\alpha} \sum_{j=0}^{N-1} a_j x^{2j+1+s} dx \\ &= \sum_{j=1}^N a_{j-1} \frac{\alpha^{2j+s}}{2j+s}, \end{aligned} \quad (2.46)$$

and observe that all sides are holomorphic and so (2.46) holds in a neighborhood of $s = -2k$. Since only the first term on the left has a pole at $-2k$, we may deduce that $\text{Res}_{(-2k)}(W_3) = a_{k-1}$. Equivalently,

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

which exposes a reflection property. \diamond

Remark 2.3.3 (W_5). Using (2.37) we may express $W_5(s)$ and $W_6(s)$ as double integrals, for example,

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

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

$$W_5(-1) = \frac{8}{\pi^4} \int_0^{\frac{\pi}{2}} \int_0^{\frac{\pi}{2}} \int_0^{\pi} \text{Re} K\left(2\sqrt{\sin^2 a + \sin^2 b + 2\sin a \sin b \cos c}\right) dc da db,$$

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

2.3.1. Elliptic integral representations. From (2.37), we derive

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

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

$$W_4(-1) = \frac{4}{\pi^3} \text{Re} \int_0^1 \int_0^1 \frac{K(x/y)}{y\sqrt{(1-x^2)(1-y^2)}} dx dy \quad (2.47)$$

$$= \frac{8}{\pi^3} \int_0^1 \int_0^1 \frac{K(t)}{\sqrt{(1-t^2y^2)(1-y^2)}} dy dt = \frac{8}{\pi^3} \int_0^1 K^2(k) dk. \quad (2.48)$$

The corresponding integral at $s = 1$ is

$$W_4(1) = \frac{32}{\pi^3} \int_0^1 \frac{(k+1)(K(k) - E(k))}{k^2} E\left(\frac{2\sqrt{k}}{k+1}\right) dk. \quad (2.49)$$

Starting with Nesterenko's theorem [153], we have

$$W_4(-1) = \frac{1}{2\pi^3} \int_{[0,1]^3} \frac{dx dy dz}{\sqrt{xyz(1-x)(1-y)(1-z)(1-x(1-yz))}}. \quad (2.50)$$

Upon computing the dx integral, followed by the change of variable $k^2 = yz$, we get:

$$W_4(-1) = \frac{1}{\pi^3} \int_0^1 \int_0^1 \frac{K(\sqrt{1-yz})}{\sqrt{yz(1-y)(1-z)}} dy dz \quad (2.51)$$

$$= \frac{2}{\pi^3} \int_0^1 \int_{k^2}^1 \frac{K(\sqrt{1-k^2})}{\sqrt{y(1-y)(y-k^2)}} dy dk = \frac{4}{\pi^3} \int_0^1 K'(k)^2 dk. \quad (2.52)$$

Compare this with the corresponding (2.47). In particular, appealing to Theorem 2.4 we derive the closed forms:

$$2 \int_0^1 K(k)^2 dk = \int_0^1 K'(k)^2 dk = \left(\frac{\pi}{2}\right)^4 {}_7F_6\left(\begin{matrix} \frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{1}{4}, 1, 1, 1, 1, 1 \end{matrix} \middle| 1\right). \quad (2.53)$$

This relation will be made more transparent in Chapter 6.

Recalling Corollary 2.2 and equation (2.31), we also deduce that

$$W_4(1) = \frac{96}{\pi^3} \int_0^1 E'(k)K'(k) dk - 8W_4(-1).$$

If we make a trigonometric change of variables in (2.51), we obtain

$$W_4(-1) = \frac{4}{\pi^3} \int_0^{\pi/2} \int_0^{\pi/2} K\left(\sqrt{1 - \sin^2 x \sin^2 y}\right) dx dy.$$

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 Conjecture 1.1:

$$W_4(-1) = \frac{1}{2} \sum_{n=0}^{\infty} \binom{-\frac{1}{2}}{n}^2 {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, -n \\ 1, 1 \end{matrix} \middle| 1\right).$$

Remark 2.3.4. Integrals of the form (2.50) are related to Beukers' integrals, which were used in the elementary derivation of the irrationality of $\zeta(3)$:

Beukers [37] showed that

$$\int_{[0,1]^3} \frac{(x(1-x)y(1-y)z(1-z))^n}{(1-(1-xy)z)^{n+1}} = \frac{A_n + B_n\zeta(3)}{d_n^3},$$

where A_n, B_n, d_n are integers and $d_n < 3^n$ is the lowest common multiple of the first n natural numbers. It is easy to bound the integral, hence

$$0 < \frac{|A_n + B_n\zeta(3)|}{d_n^3} < 3(\sqrt{2} - 1)^{4n}.$$

Therefore $0 < |A_n + B_n\zeta(3)| < \left(\frac{4}{5}\right)^n$, implying irrationality.

We revisit such integrals in Chapter 6, some of which also evaluate to $\zeta(3)$, but the bounds for their integrands are too poor. \diamond

Remark 2.3.5 (Watson integrals). From the evaluation (2.4) we note that $W_3(-1)$ is twice the value of one of the triple integrals considered by Watson in [194]:

$$W_3(-1) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{dudvdw}{3 - \cos v \cos w - \cos w \cos u - \cos u \cos v}. \quad (2.54)$$

This is derived in [44] and various related extensions are found in [20].

Watson's integral (2.54) also gives the alternative representation:

$$W_3(-1) = \pi^{-5/2} G_{3,3}^{3,2} \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 0, 0, 0 \end{matrix} \middle| 4 \right). \quad (2.55)$$

The equivalence of this and the Meijer G representation coming from Theorem 2.2 can be established similarly to the proof of Theorem 2.4, upon using the transformation (2.29). \diamond

Remark 2.3.6 (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

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

Appealing to (2.44) we deduce that

$$\sum_{k=0}^{\infty} \frac{W_3(2k)}{9^k(k+1)} = \frac{\sqrt{3}\pi}{4}. \quad (2.56)$$

In fact, as Kluyver shows in [123], the probability of an n -step walk ending in the unit disk is $1/(n+1)$. This is obtained by setting $\alpha = 1$ in (2.5). See also [33] for a very short proof of this fact; the amazing proof uses not much more than the sum of angles in a triangle. Moreover, [33] gives an extension: for two walkers starting at the origin, who take m and n steps respectively, the probability that the first walker ends up further than the second walker is $m/(m+n)$ (for $m = 1$ we recover Kluyver's result; the $m = n$ case is obvious). In terms of integrals, this gives the non-trivial identity

$$\int_0^m P_n(x) p_m(x) dx = \frac{m}{m+n}.$$

One example of such an integral is (using p_3 from Chapter 3)

$$\int_0^2 \frac{4\sqrt{3}x \cos^{-1}\left(\frac{x}{2}\right)}{\pi^2(3+x^2)} {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \mid \frac{x^2(9-x^2)^2}{(3+x^2)^3}\right) dx = \frac{2}{5}.$$

◇

2.4. Partial resolution of the conjecture

We may now investigate Conjecture 1.1 which states, for positive integers n and complex s ,

$$W_{2n}(s) \stackrel{?}{=} \sum_{j \geq 0} \binom{s/2}{j}^2 W_{2n-1}(s-2j). \quad (2.57)$$

We can resolve this conjecture modulo a technical estimate given in Conjecture 2.2. The proof outline below explains the conjecture by identifying the terms of the infinite sum as natural residues.

PROOF. Using (2.8) we write W_{2n} as a Bessel integral

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

Then we apply Theorem 2.1 to $J_0^{2n} = J_0^{2n-1} \cdot J_0$ for s in a vertical strip. Since, again by (2.8), we have

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

we obtain

$$\begin{aligned} W_{2n}(-s) &= 2^{1-s} \frac{\Gamma(1-s/2)}{\Gamma(s/2)} \int_0^\infty x^{s-1} J_0^{2n-1}(x) \cdot J_0(x) dx \\ &= \frac{\Gamma(1-s/2)}{\Gamma(s/2)} \frac{1}{2\pi i} \int_{\delta-i\infty}^{\delta+i\infty} \frac{1}{2} \frac{\Gamma(z/2)\Gamma(s/2-z/2)}{\Gamma(1-z/2)\Gamma(1-s/2+z/2)} W_{2n-1}(-z) dz \end{aligned} \quad (2.58)$$

where $0 < \delta < 1$.

Observe that the integrand has poles at $z = s, s+2, s+4, \dots$ coming from $\Gamma(s/2 - z/2)$. On the other hand, the term $W_{2n-1}(-z)$ has at most simple poles at $z = 2, 4, 6, \dots$ which are canceled by the corresponding zeros of $\Gamma(1 - z/2)$. This asserted pole structure of W_{2n-1} was shown in Example 2.2.3 for $n = 3$ and may be shown analogously for each $n = 4, 5, \dots$ based on Proposition 2.1.

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

$$W_{2n}(-s) = \sum_{j \geq 0} \binom{-s/2}{j}^2 W_{2n-1}(-s - 2j), \quad (2.59)$$

which is what we want to prove, provided that the contour of the integral after (2.58) can be closed in the right half-plane. \square

This proof is thus rigorous provided that the next two conjectures hold. Conjecture 2.1 is easily checked for individual n .

Conjecture 2.1 (Poles of W_{2n-1}). *For each $n \geq 1$ all poles of W_{2n-1} are simple.*

Conjecture 2.2 (Growth of W_{2n-1}). *For given s ,*

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

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

Remark 2.4.1 (Other approaches to Conjecture 2.57). We restrict ourself to the core case with $n = 2$. One can prove using creative telescoping 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 (2.6) and ignoring the restriction on s ,

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

on appealing to Example 2.2.1, since for $x > 0$

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

There is a corresponding (formal) manipulation for $s = 1$. In Chapter 3, we rigorously prove the conjecture for $n = 2$ and s an integer. \diamond

CHAPTER 3

Densities of Short Uniform Random Walks

ABSTRACT. We continue our study of the densities of uniform random walks in the plane, focusing on three and four steps, and less so on five steps. As a main result, we obtain a hypergeometric representation of the density for four steps. It appears unrealistic to expect similar results for more than five steps. New results are also presented concerning the moments of the walks. Relations with Mahler measures are discussed.

3.1. Introduction

Recall that 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 in a uniformly random direction. The study of such walks largely originated with Pearson more than a century ago [159, 160, 158] who posed the problem of determining the distribution of the distance from the origin after a certain number of steps. Here we study the (radial) densities p_n of the distance from the origin after n steps. This continues research commenced in [53, 56] (Chapters 1, 2) where the focus was on the moments of these distributions:

$$W_n(s) := \int_0^n p_n(t) t^s dt.$$

The densities for walks of up to 8 steps are depicted in Figure 1. As established by Lord Rayleigh [165], p_n quickly approaches the probability density $\frac{2x}{n} e^{-x^2/n}$ for large n . This limiting density is superimposed in Figure 1 for $n \geq 5$.

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

$$p_2(x) = \frac{2}{\pi\sqrt{4-x^2}} \tag{3.1}$$

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

$$p_3(x) = \operatorname{Re} \frac{\sqrt{x}}{\pi^2} K \left(\sqrt{\frac{(x+1)^3(3-x)}{16x}} \right). \tag{3.2}$$

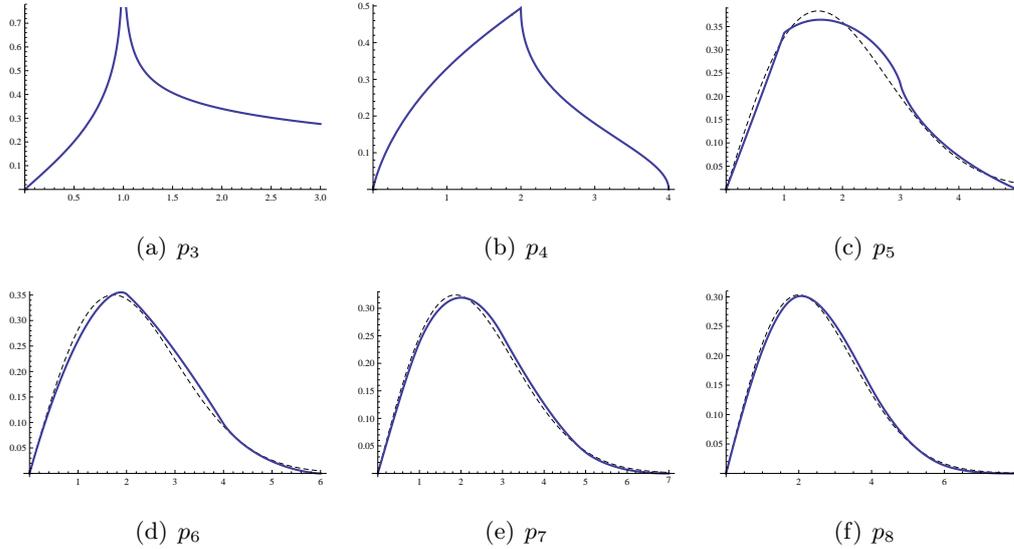


FIGURE 1. Densities p_n with the limiting behaviour superimposed for $n \geq 5$.

One of the main results of this chapter is a closed form evaluation of p_4 as a hypergeometric function given in Theorem 3.6. In (3.17) we also provide a single hypergeometric closed form for p_3 which, in contrast to (3.2), is real and valid on all of $[0, 3]$. For convenience, we list these two closed forms here:

$$p_3(x) = \frac{2\sqrt{3}}{\pi} \frac{x}{(3+x^2)} {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \middle| \frac{x^2(9-x^2)^2}{(3+x^2)^3}\right), \quad (3.3)$$

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16-x^2}}{x} \operatorname{Re} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{(16-x^2)^3}{108x^4}\right). \quad (3.4)$$

A striking feature of the 3- and 4-step densities is their *modularity*. It is this circumstance which allows us to express them via hypergeometric series; we will continue our study of modular functions in Chapters 10 and 11.

In Section 3.2 we give general results for the densities p_n and prove that they satisfy certain linear differential equations. In Sections 3.3 – 3.5 we provide special results for p_3 , p_4 , and p_5 . Particular interest is taken in the behaviour near the points where the densities fail to be smooth. In Section 3.6 we study the derivatives of the moment function and make a connection to multidimensional *Mahler measures*. Finally in Section 3.7 we provide some related new evaluations of moments and so resolve a central case of the conjecture in Chapter 1.

We close this introduction with a historical remark illustrating the fascination arising from these densities. H. Fettis devotes the entire paper [92] to proving that p_5 is not linear on the initial interval $[0, 1]$ as ruminated upon by Pearson [158]. This will be explained in Section 3.5.

3.2. The densities p_n

It is a classical result of Kluyver [123] that p_n has the following Bessel integral representation:

$$p_n(x) = \int_0^\infty xtJ_0(xt)J_0^n(t) dt. \quad (3.5)$$

It is visually clear from the graphs in Figure 1 that p_n is getting smoother for increasing n . This can be made precise from (3.5) using the asymptotic formula for J_0 for large arguments [155] and dominated convergence:

Proposition 3.1. *For each integer $n \geq 0$, the density p_{n+4} is $\lfloor n/2 \rfloor$ times continuously differentiable.*

We note from Figure 1 that the only points preventing p_n from being smooth appear to be integers. This will be made precise in Theorem 3.1.

We recall a few things about the s th moments $W_n(s)$ of the density p_n which are given by

$$W_n(s) = \int_0^\infty x^s p_n(x) dx = \int_{[0,1]^n} \left| \sum_{k=1}^n e^{2\pi x_k i} \right|^s d\mathbf{x}. \quad (3.6)$$

It was shown in Chapter 1 and 2 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 $s = -2, -4, -6, \dots$ and $W_4(s)$ has double poles at these integers.

Moreover, from the combinatorial evaluation

$$W_n(2k) = \sum_{a_1 + \dots + a_n = k} \binom{k}{a_1, \dots, a_n}^2 \quad (3.7)$$

it followed that $W_n(s)$ satisfies a functional equation, coming from the inevitable recursion that exists for the right-hand side of (3.7), see e. g. (3.8).

The first part of equation (3.6) can be rephrased as saying that $W_n(s-1)$ is the *Mellin transform* of p_n [150]. We denote this by $W_n(s-1) = \mathcal{M}[p_n; s]$. Conversely, the density p_n is the *inverse Mellin transform* of $W_n(s-1)$. We intend to exploit this relation as detailed for $n = 4$ in the following example.

Example 3.2.1 (Mellin transform). For $n = 4$, the moments $W_4(s)$ satisfy the functional equation

$$(s+4)^3 W_4(s+4) - 4(s+3)(5s^2 + 30s + 48)W_4(s+2) + 64(s+2)^3 W_4(s) = 0. \quad (3.8)$$

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

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

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 (3.8) of W_4 into the differential equation $A_4 \cdot p_4(x) = 0$ where A_4 is the operator

$$A_4 = x^4(\theta + 1)^3 - 4x^2\theta(5\theta^2 + 3) + 64(\theta - 1)^3 \quad (3.9)$$

$$\begin{aligned} &= (x - 4)(x - 2)x^3(x + 2)(x + 4)D_x^3 + 6x^4(x^2 - 10)D_x^2 \\ &\quad + x(7x^4 - 32x^2 + 64)D_x + (x^2 - 8)(x^2 + 8), \end{aligned} \quad (3.10)$$

where $\theta = xD_x$. 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 $x \rightarrow 4^-$ (see Theorem 3.3) 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. \diamond

Theorem 3.1. *Let an integer $n \geq 1$ 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 3.2.1, 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 [150]. 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 Chapter 1.

The leading coefficient of the differential equation (in terms of D_x as in (3.10)) turns out to be

$$x^{n-1} \prod_{2|(m-n)} (x^2 - m^2) \quad (3.11)$$

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 3.2.1.

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 [116, 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. \square

Remark 3.2.1. It is a basic property of the Mellin transform, see for instance [94, 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. Since 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 3.4.1.

3.2.1. An explicit recursion. We close this section by providing details for the claim made in (3.11). 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 $n - 1$. An entirely explicit formula for this recurrence is given in [189], see Theorem 1.1.

Observe that (3.11) is easily checked for each fixed n by applying Theorem 1.1. We explicitly checked the cases $n \leq 1000$. The fact that (3.11) is true in general is recorded in Theorem 3.2 below.

For fixed n , write the recurrence for $f_n(k)$ in the form $\sum_{j=0}^{n-1} k^j q_j(K)$ where q_j are polynomials and K is the shift $k \rightarrow k + 1$. Then q_{n-1} is the characteristic polynomial of this recurrence, and, by the rules in Example 3.2.1, we find that the differential equation satisfied by $p_n(x)$ is of the form $q_{n-1}(x^2)\theta^{n-1} +$ lower order terms in θ .

We claim that the characteristic polynomial of the recurrence in Theorem 1.1 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 (3.11). By Theorem 1.1 the characteristic polynomial is

$$\sum_{j=0}^{\lambda} \left[\sum_{\alpha_1, \dots, \alpha_j} \prod_{i=1}^j (-\alpha_i)(n+1-\alpha_i) \right] x^{\lambda-j} \quad (3.12)$$

where $\lambda = \lceil n/2 \rceil$ and the sum is again over all sequences $\alpha_1, \dots, \alpha_j$ such that $0 \leq \alpha_i \leq n$ and $\alpha_{i+1} \leq \alpha_i - 2$. The claimed evaluation is thus equivalent to the identity in the theorem below, first proven by P. Djakov and B. Mityagin [86], and communicated to us by D. Zagier. Zagier also gives a very neat and purely combinatorial proof [57], which uses experimental mathematics, and the key step involves inserting a dummy variable and finding a recursion in terms of that variable. Another combinatorial proof is given in [173].

Theorem 3.2. *For all integers $n, j \geq 1$,*

$$\sum_{\substack{0 \leq m_1, \dots, m_j < n/2 \\ m_i < m_{i+1}}} \prod_{i=1}^j (n - 2m_i)^2 = \sum_{\substack{1 \leq \alpha_1, \dots, \alpha_j \leq n \\ \alpha_i < \alpha_{i+1} - 2}} \prod_{i=1}^j \alpha_i (n + 1 - \alpha_i). \quad (3.13)$$

3.3. The density p_3

The elliptic integral evaluation (3.2) of p_3 is suitable for extracting information about the features of p_3 exposed in Figure 1. It follows, for instance, that p_3 has a singularity at 1. Moreover, using the known asymptotics for $K(x)$ [46, Ch. 1], we may deduce that the singularity is of the form

$$p_3(x) = \frac{3}{2\pi^2} \log \left(\frac{4}{|x-1|} \right) + O(1) \quad (3.14)$$

as $x \rightarrow 1$.

We also recall from Chapter 2 that p_3 has the expansion, valid for $0 \leq x \leq 1$,

$$p_3(x) = \frac{2x}{\pi\sqrt{3}} \sum_{k=0}^{\infty} W_3(2k) \left(\frac{x}{3} \right)^{2k} \quad (3.15)$$

where

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

is the sum of squares of trinomials. The following functional relation holds,

$$p_3(x) = \frac{4x}{(3-x)(x+1)} p_3 \left(\frac{3-x}{1+x} \right), \quad (3.16)$$

so that (3.15) 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 3.3.1 (Hypergeometric form for p_3). Using the techniques in [75] we can deduce from (3.15) that

$$p_3(x) = \frac{2\sqrt{3}x}{\pi(3+x^2)} {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \middle| \frac{x^2(9-x^2)^2}{(3+x^2)^3}\right), \quad (3.17)$$

which is found in a similar way to the hypergeometric form of p_4 given in Theorem 3.6. Once obtained, this identity is easily proven using the differential equation from Theorem 3.1 satisfied by p_3 (note that the right hand side satisfies a modification of the hypergeometric differential equation, (14.3)) – as is typical in experimental mathematics. From (3.17) we see, for example, that $p_3(\sqrt{3})^2 = \frac{3}{2\pi^2}W_3(-1)$. \diamond

Example 3.3.2 (Iterative form for p_3). The expression (3.17) can be interpreted in terms of the cubic AGM, AG_3 [45]. Recall that $\text{AG}_3(a, b)$ 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,

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

so we have, for $0 \leq x \leq 3$,

$$p_3(x) = \frac{2\sqrt{3}}{\pi} \frac{x}{\text{AG}_3(3+x^2, 3|1-x^2|^{2/3})}. \quad (3.18)$$

\diamond

3.4. The density p_4

The densities p_n are recursively related. As in [118], setting $\phi_n(x) = p_n(x)/(2\pi x)$, we have for integers $n \geq 2$

$$\phi_n(x) = \frac{1}{2\pi} \int_0^{2\pi} \phi_{n-1}(\sqrt{x^2 - 2x \cos \alpha + 1}) d\alpha. \quad (3.19)$$

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

Theorem 3.3. *As $x \rightarrow 4^-$,*

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

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

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

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

$$\phi_4'(x) = -\frac{1}{\pi} \frac{(x^2+8)\phi_3(3)}{x\sqrt{(16-x^2)(x^2-4)}} + \frac{1}{\pi} \int_0^{\arccos\left(\frac{x^2-8}{2x}\right)} (x - \cos(\alpha)) \frac{\phi_3'(y)}{y} d\alpha. \quad (3.20)$$

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

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

Here, we used $\phi_3(3) = \frac{\sqrt{3}}{12\pi^2}$. 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 (3.20) twice more proves the claim. \square

Remark 3.4.1. The situation for the singularity at $x = 2^+$ is more complicated since in (3.20) both the integral (via the logarithmic singularity of ϕ_3 at 1, see (3.14)) and the boundary term contribute. Numerically, we find, as $x \rightarrow 2^+$,

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

The derivative of p_4 at 2 from the left is quite marvelously given by

$$p_4'(2^-) = \frac{1}{2\sqrt{3}\pi} W_3(1), \quad (3.21)$$

compare with (3.29). These observations can be proven in hindsight from Theorem 3.5; the latter makes use of contiguous relations found in Chapter 14. \diamond

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 3.2.1.

Example 3.4.1. From Chapter 2, we know that W_4 has a pole of order 2 at -2 as illustrated in Figure 2(b) of Chapter 1. More specifically, results in Section 3.6 give

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

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

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

as $x \rightarrow 0$. ◇

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

$$W_4(s) = \frac{s_{4,k-1}}{(s+2k)^2} + \frac{r_{4,k-1}}{s+2k} + O(1) \quad (3.22)$$

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

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

In fact, knowing that p_4 solves the linear Fuchsian differential equation (3.9) with a regular singularity at 0, we may conclude:

Theorem 3.4. *For small values $x > 0$,*

$$p_4(x) = \sum_{k=0}^{\infty} (r_{4,k} - s_{4,k} \log(x)) x^{2k+1}. \quad (3.23)$$

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 (this is a common technique used in many of our proofs). The numbers $W_4(2k)$ are also known as the Domb numbers [20], and their hypergeometric generating function is given in [171] and has been further studied in [75]. We thus have

$$\sum_{k=0}^{\infty} s_{4,k} x^{2k+1} = \frac{6x}{\pi^2 (4-x^2)} {}_3F_2 \left(\begin{matrix} \frac{1}{3}, \frac{1}{2}, \frac{2}{3} \\ 1, 1 \end{matrix} \middle| \frac{108x^2}{(x^2-4)^3} \right) \quad (3.24)$$

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

For future use, we note that (3.24) can also be written as

$$\sum_{k=0}^{\infty} s_{4,k} x^{2k+1} = \frac{24x}{\pi^2 (16-x^2)} {}_3F_2 \left(\begin{matrix} \frac{1}{3}, \frac{1}{2}, \frac{2}{3} \\ 1, 1 \end{matrix} \middle| \frac{108x^4}{(16-x^2)^3} \right) \quad (3.25)$$

which follows from the transformation

$$(1-4x)_3F_2\left(\frac{1}{3}, \frac{1}{2}, \frac{2}{3} \middle| -\frac{108x}{(1-16x)^3}\right) = (1-16x)_3F_2\left(\frac{1}{3}, \frac{1}{2}, \frac{2}{3} \middle| \frac{108x^2}{(1-4x)^3}\right) \quad (3.26)$$

given in [75, (3.1)].

On the other hand, as a consequence of (3.22) and the functional equation (3.8) satisfied by W_4 , the residues $r_{4,k}$ can be obtained from the recurrence relation

$$\begin{aligned} 128k^3r_{4,k} &= 4(2k-1)(5k^2-5k+2)r_{4,k-1} - 2(k-1)^3r_{4,k-2} \\ &\quad + 3(64k^2s_{4,k} - (20k^2-20k+6)s_{4,k-1} + (k-1)^2s_{4,k-2}) \end{aligned} \quad (3.27)$$

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

Remark 3.4.2. In fact, before realising 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 s 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 3.4.

The accidental discovery of the required form was amusing and we recount it here. Interested in plotting $p_4'(x)$ for small x , the author resorted to the most numerically stable method available then – (2.40) and derivation using first principles. However, instead of using the correct derivative formula

$$\lim_{h \rightarrow 0} \frac{p_4(x+h) - p_4(x)}{h},$$

a typographical error was made and the following formula was used instead:

$$\lim_{h \rightarrow 0} \frac{p_4(x+h) - p_4(h)}{x}.$$

Upon correcting the mistake, it was noticed, amazingly, that the two plots produced were almost exactly related by a vertical translation of 0.14 units. This means that p_4 ‘almost’ satisfies a differential equation

$$f'(x) + a = \frac{f(x)}{x},$$

whose solution is $f(x) = bx - ax \log x$, where $a \approx 0.14$ and $b \approx 0.33$ (since $\int_0^1 f(x) dx = \frac{1}{5}$). The log form of p_4 , and the numerical connection between a, b and the coefficients of the poles, then became apparent. \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 [119]. Since the indicial equation has 1 as a triple root, the solution (3.24) 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 (3.32), and from (3.23), 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. After much work, a hypergeometric representation of p_4 with rational argument is possible.

Theorem 3.5. *For $2 < x < 4$,*

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16-x^2}}{x} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{(16-x^2)^3}{108x^4}\right). \quad (3.28)$$

PROOF. Denote the right-hand side of (3.28) 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 (3.9), which is also satisfied by p_4 as proven in Theorem 3.1. Together with the boundary conditions supplied by Theorem 3.3 it follows that $p_4 = q_4$. \square

We note that Theorem 3.5 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 3.3. We also get the evaluation

$$p_4(2) = \frac{2^{7/3}\pi}{3\sqrt{3}\Gamma^6(2/3)} = \frac{\sqrt{3}}{\pi} W_3(-1). \quad (3.29)$$

Quite marvelously, as first discovered numerically:

Theorem 3.6. *For $0 < x < 4$,*

$$p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16-x^2}}{x} \operatorname{Re} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{(16-x^2)^3}{108x^4}\right). \quad (3.30)$$

PROOF. To obtain the analytic continuation of the ${}_3F_2$ for $0 < x < 2$ we employ the formula [136, (5.3)], valid for all z ,

$$\begin{aligned} {}_{q+1}F_q \left(\begin{matrix} a_1, \dots, a_{q+1} \\ b_1, \dots, b_q \end{matrix} \middle| z \right) &= \frac{\prod_j \Gamma(b_j)}{\prod_j \Gamma(a_j)} \sum_{k=1}^{q+1} \frac{\Gamma(a_k) \prod_{j \neq k} \Gamma(a_j - a_k)}{\prod_j \Gamma(b_j - a_k)} (-z)^{-a_k} \\ &\quad \times {}_{q+1}F_q \left(\begin{matrix} a_k, \{a_k - b_j + 1\}_{j \neq k} \\ \{a_k - a_j + 1\}_{j \neq k} \end{matrix} \middle| \frac{1}{z} \right), \end{aligned} \quad (3.31)$$

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

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

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

$$\begin{aligned} \operatorname{Re} {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \middle| z \right) &= \frac{\log(108z)}{2\sqrt{3z}} {}_3F_2 \left(\begin{matrix} \frac{1}{3}, \frac{1}{2}, \frac{2}{3} \\ 1, 1 \end{matrix} \middle| \frac{1}{z} \right) \\ &\quad + \frac{1}{2\sqrt{3z}} \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{1}{2})_n (\frac{2}{3})_n}{n!^3} \left(\frac{1}{z} \right)^n (5H_n - 2H_{2n} - 3H_{3n}). \end{aligned} \quad (3.32)$$

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

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

we thus find that the right-hand side of (3.30) is given by $-\log(x)S_4(x)$ plus

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

where S_4 is the solution to the differential equation for p_4 given in (3.25). 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 3.4 this proves the claim. \square

Remark 3.4.3. Let us indicate how the hypergeometric expression for p_4 given in Theorem 3.5 was discovered. Consider the generating series

$$y_0(z) = \sum_{k=0}^{\infty} W_4(2k)z^k \quad (3.33)$$

which is just a rescaled version of (3.24). Corresponding to (3.25), the hypergeometric form for this series is

$$y_0(z) = \frac{1}{1-4z} {}_3F_2 \left(\begin{matrix} \frac{1}{3}, \frac{1}{2}, \frac{2}{3} \\ 1, 1 \end{matrix} \middle| \frac{108z^2}{(1-4z)^3} \right) \quad (3.34)$$

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

$$B_4 = 64z^2(\theta + 1)^3 - 2z(2\theta + 1)(5\theta^2 + 5\theta + 2) + \theta^3. \quad (3.35)$$

Up to a change of variables this is (3.9); y_0 is the unique solution which is analytic at zero and takes the value 1 at zero; the other solutions have a single or double logarithmic singularity. Let y_1 be the solution characterised by

$$y_1(z) - y_0(z) \log(z) \in z\mathbb{Q}[[z]]. \quad (3.36)$$

Note that it follows from (3.36), as well as Theorem 3.4 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

$$p_4(x) = -\frac{3x}{4\pi^2} y_1\left(\frac{x^2}{64}\right). \quad (3.37)$$

If $x \in (2, 4)$ and $z = x^2/64$ then the argument $t = \frac{108z^2}{(1-4z)^3}$ in (3.34) takes values in $(1, \infty)$. We therefore consider the solutions of the corresponding hypergeometric equation at infinity. A standard basis for these is

$$t^{-1/3} {}_3F_2\left(\begin{matrix} \frac{1}{3}, \frac{1}{3}, \frac{1}{3} \\ \frac{2}{3}, \frac{5}{6} \end{matrix} \middle| \frac{1}{t}\right), \quad t^{-1/2} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \middle| \frac{1}{t}\right), \quad t^{-2/3} {}_3F_2\left(\begin{matrix} \frac{2}{3}, \frac{2}{3}, \frac{2}{3} \\ \frac{4}{3}, \frac{7}{6} \end{matrix} \middle| \frac{1}{t}\right). \quad (3.38)$$

In fact, the second element suffices to express p_4 on the interval $(2, 4)$ as shown in Theorem 3.5. \diamond

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

Remark 3.4.4. As shown in [75], the series y_0 defined in (3.33) possesses the modular parameterisation

$$y_0\left(-\frac{\eta(2\tau)^6\eta(6\tau)^6}{\eta(\tau)^6\eta(3\tau)^6}\right) = \frac{\eta(\tau)^4\eta(3\tau)^4}{\eta(2\tau)^2\eta(6\tau)^2}. \quad (3.39)$$

Here η is the *Dedekind eta function* defined as

$$\eta(\tau) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n) = q^{1/24} \sum_{n=-\infty}^{\infty} (-1)^n q^{n(3n+1)/2}, \quad (3.40)$$

where $q = e^{2\pi i\tau}$. Moreover, the quotient of the logarithmic solution y_1 defined in (3.36) and y_0 are related by

$$\exp\left(\frac{y_1(z)}{y_0(z)}\right) = e^{(2\tau+1)\pi i} = -q. \quad (3.41)$$

Combining (3.39), (3.41) and (3.37), one obtains the modular representation

$$p_4 \left(8i \frac{\eta(2\tau)^3 \eta(6\tau)^3}{\eta(\tau)^3 \eta(3\tau)^3} \right) = \frac{6(2\tau + 1)}{\pi} \eta(\tau) \eta(2\tau) \eta(3\tau) \eta(6\tau), \quad (3.42)$$

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 (5/3)rd singular value of the next section). As a consequence, the value $p_4(1)$ has a nice evaluation which is given in Theorem 3.7. \diamond

3.5. The density p_5

As shown in Chapter 2, $W_5(s)$ has simple poles at $-2, -4, \dots$, compare Figure 2(c) in Chapter 1. We write $r_{5,k} = \text{Res}_{-2k-2} W_5$ for the residue of W_5 at $s = -2k-2$. A surprising bonus is the evaluation of $r_{5,0} = p_4(1) \approx 0.3299338011$, the residue at $s = -2$. This is because in general for $n \geq 4$, one has

$$\text{Res}_{-2} W_{n+1} = p'_{n+1}(0) = p_n(1), \quad (3.43)$$

as follows from Proposition 2.1; here p'_n denotes the derivative from the right.

Explicitly, using Theorem 3.6, we have,

$$r_{5,0} = p'_5(0) = \frac{2\sqrt{15}}{\pi^2} \text{Re } {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{5}{6}, \frac{7}{6} \end{matrix} \middle| \frac{125}{4} \right),$$

from which we get

$$r_{5,0} = \frac{\sqrt{5/3}}{\pi} {}_2F_1 \left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| \frac{1 - \sqrt{5}}{2} \right)^2, \quad (3.44)$$

using Clausen's formula [11, p. 116] and a quadratic transformation.

Based on the modularity of p_4 discussed in Remark 3.4.4, we find:

Theorem 3.7.

$$\begin{aligned} r_{5,0} &= \frac{\sqrt{5}}{40} \frac{\Gamma(\frac{1}{15})\Gamma(\frac{2}{15})\Gamma(\frac{4}{15})\Gamma(\frac{8}{15})}{\pi^4} \\ &= \frac{3\sqrt{5}}{\pi^3} \frac{(\sqrt{5} - 1)}{2} K_{15}^2 = \frac{\sqrt{15}}{\pi^3} K_{5/3} K_{15}, \end{aligned} \quad (3.45)$$

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

PROOF. Let $\phi = (\sqrt{5} - 1)/2$ (the golden ratio). In the notation of Section 10.2, it can be verified that the value $\tau = \frac{i}{\sqrt{3}} {}_2F_1(\frac{1}{3}, \frac{2}{3}; 1; 1 + \phi)/{}_2F_1(\frac{1}{3}, \frac{2}{3}; 1; -\phi)$ is a quadratic irrationality (it being $(1 + \sqrt{-5/3})/2$). As such, it is known that ${}_2F_1(\frac{1}{3}, \frac{2}{3}; 1; -\phi)$ may be effectively computed in terms of algebraic numbers and Gamma functions by the Chowla–Selberg formula [175]. A proof with every minute detail attended to has been written down (A. Straub, private communication, July 2012). \square

Remarkably, these evaluations appear to extend to $r_{5,1} \approx 0.006616730259$, the residue at $s = -4$. We discovered and checked to 400 places using (3.51) and (3.52) that

$$r_{5,1} \stackrel{?}{=} \frac{13}{225} r_{5,0} - \frac{2}{5\pi^4} \frac{1}{r_{5,0}}. \quad (3.46)$$

We summarise our knowledge as follows:

Theorem 3.8. *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*

$$\begin{aligned} A_5 = & x^6(\theta + 1)^4 - x^4(35\theta^4 + 42\theta^2 + 3) \\ & + x^2(259(\theta - 1)^4 + 104(\theta - 1)^2) - (15(\theta - 3)(\theta - 1))^2. \end{aligned} \quad (3.47)$$

Moreover, for small $x > 0$,

$$p_5(x) = \sum_{k=0}^{\infty} r_{5,k} x^{2k+1}, \quad \text{where} \quad (3.48)$$

$$\begin{aligned} (15(2k+2)(2k+4))^2 r_{5,k+2} = & (259(2k+2)^4 + 104(2k+2)^2) r_{5,k+1} \\ & - (35(2k+1)^4 + 42(2k+1)^2 + 3) r_{5,k} + (2k)^4 r_{5,k-1} \end{aligned} \quad (3.49)$$

with explicit initial values $r_{5,-1} = 0$ and $r_{5,0}, r_{5,1}$ given by (3.45) and (3.46).

PROOF. First, the differential equation (3.47) is computed as was that for p_4 . Next, as detailed in Chapter 2, the residues satisfy the recurrence relation (3.49) with the given initial values. Finally, proceeding as for (3.23), we deduce that (3.48) holds for small $x > 0$. \square

Numerically, the series (3.48) appears to converge for $|x| < 3$ which is in accordance with $\frac{1}{9}$ being a root of the characteristic polynomial of the recurrence (3.49).

Since the poles of W_5 are simple, no logarithmic terms are involved in (3.48). In particular, by computing a few more residues from (3.49),

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

near 0, explaining the strikingly straight shape of $p_5(x)$ on $[0, 1]$ – see Figure 1 (c). This phenomenon was observed by Pearson [158] 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...”

This conjecture was investigated in [92] where the nonlinearity was first rigorously established. The difficulty of computing the underlying Bessel integrals is hence manifest.

Remark 3.5.1. The moments W_3, W_4, W_5 , as well as the Apéry-like sequences studied in Chapter 11, are closely related to solutions of Calabi-Yau type differential equations [8], which can be identified with differential equations for the periods of Calabi-Yau manifolds in theoretical physics. For example, the generating function for $W_5(2k)$ is an analytic solution of equation 34 tabulated in [7]. \diamond

3.6. Derivative evaluations of W_n

As illustrated by Theorem 3.4, 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 3.6.1 (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

$$\text{Res}_{-2}(W_3) = \frac{8 + 12W'_3(0) - 4W'_3(2)}{9}. \quad (3.50)$$

This works in general and we likewise obtain:

$$\text{Res}_{-2}(W_5) = \frac{16 + 1140W'_5(0) - 804W'_5(2) + 64W'_5(4)}{225}, \quad (3.51)$$

$$\text{Res}_{-4}(W_5) = \frac{26 \text{Res}_{-2}(W_5) - 16 - 20W'_5(0) + 4W'_5(2)}{225}. \quad (3.52)$$

In the presence of double poles, as for W_4 ,

$$\lim_{s \rightarrow -2} (s+2)^2 W_4(s) = \frac{3 + 4W_4'(0) - W_4'(2)}{8} \quad (3.53)$$

and for the residue:

$$\text{Res}_{-2}(W_4) = \frac{9 + 18W_4'(0) - 3W_4'(2) + 4W_4''(0) - W_4''(2)}{16}. \quad (3.54)$$

Equations (3.53, 3.54) are used in Example 3.4.1 and each unknown is evaluated below. \diamond

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

Example 3.6.2 (Derivatives of W_3 and W_4). Differentiating the double integral for $W_3(s)$ (3.6) under the integral sign, we have

$$\begin{aligned} W_3'(0) &= \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \log(3 + 2 \cos x + 2 \cos y + 2 \cos(x-y)) \, dx \, dy \\ &= \frac{1}{2} \int_0^1 \int_0^1 \log(4 \sin(\pi y) \cos(2\pi x) + 3 - 2 \cos(2\pi y)) \, dx \, dy. \end{aligned} \quad (3.55)$$

Then, using

$$\int_0^1 \log(a + b \cos(2\pi x)) \, dx = \log \frac{a + \sqrt{a^2 - b^2}}{2} \quad \text{for } a > b > 0, \quad (3.56)$$

we deduce

$$W_3'(0) = \int_{1/6}^{5/6} \log(2 \sin(\pi y)) \, dy = \frac{1}{\pi} \text{Cl}\left(\frac{\pi}{3}\right), \quad (3.57)$$

where Cl denotes the *Clausen* function, given by

$$\text{Cl}(t) = \sum_{n=1}^{\infty} \frac{\sin(nt)}{n^2} = - \int_0^t \log \left| 2 \sin \frac{x}{2} \right| \, dx. \quad (3.58)$$

Knowing that the residue at $s = -2$ is $2/(\sqrt{3}\pi)$, we can also obtain from (3.50)

$$W_3'(2) = 2 + \frac{3}{\pi} \text{Cl}\left(\frac{\pi}{3}\right) - \frac{3\sqrt{3}}{2\pi}.$$

In like fashion,

$$\begin{aligned} W_4'(0) &= \frac{3}{2} \int_0^{\frac{1}{2}} \int_0^{\frac{1}{2}} \log((1 + \cos(2\pi x) + \cos(2\pi y))^2 + (\sin(2\pi x) + \sin(2\pi y))^2) \, dx \, dy \\ &= \frac{3}{8\pi^2} \int_0^{\pi} \int_0^{\pi} \log(3 + 2 \cos x + 2 \cos y + 2 \cos(x-y)) \, dx \, dy \\ &= \frac{7}{2} \frac{\zeta(3)}{\pi^2}. \end{aligned} \quad (3.59)$$

The final equality will be shown in Example 3.6.3.

The superficial similarity between $W'_3(0)$ in (3.55) and $W'_4(0)$ in (3.59) comes from applying the formula (see Chapter 8)

$$\int_0^1 \log((a + \cos 2\pi x)^2 + (b + \sin 2\pi x)^2) dx = \begin{cases} \log(a^2 + b^2) & \text{if } a^2 + b^2 > 1, \\ 0 & \text{otherwise} \end{cases}$$

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.)

The factor of 3 in the numerator of (3.59) can be explained: after applying the reduction above and symmetry, we are actually required to evaluate the first double integral in (3.59) in the region bounded by $y = x + 1/2$, $y = 0$, $y = 1/2$ and $x = 1/2$. This region splits into a right isosceles triangle and a square; let the value of the integral be I_b and I_a in them respectively. Now, in the region bounded by $y = x + 1/2$, $y = x$, $y = 0$, and $y = 1/2$ (i. e. I_b and half of I_a), the transformation $x \mapsto y - x$ leaves the integrand invariant but maps the region into a ; thus $I_b = I_a/2$, and on the whole region the integral has value $3I_a/2$. \diamond

Remark 3.6.1. In general, differentiating the Bessel integral expression [65]

$$W_n(s) = 2^{s+1-k} \frac{\Gamma(1 + \frac{s}{2})}{\Gamma(k - \frac{s}{2})} \int_0^\infty x^{2k-s-1} \left(-\frac{1}{x} \frac{d}{dx}\right)^k J_0^n(x) dx, \quad (3.60)$$

under the integral sign gives

$$\begin{aligned} W'_n(0) &= n \int_0^\infty \left(\log\left(\frac{2}{x}\right) - \gamma\right) J_0^{n-1}(x) J_1(x) dx \\ &= \log(2) - \gamma - n \int_0^\infty \log(x) J_0^{n-1}(x) J_1(x) dx, \end{aligned} \quad (3.61)$$

where γ is the *Euler-Mascheroni* constant (a novel method for the computation of which can be found in Section 14.3), and

$$W''_n(0) = n \int_0^\infty \left(\log\left(\frac{2}{x}\right) - \gamma\right)^2 J_0^{n-1}(x) J_1(x) dx.$$

Likewise

$$\begin{aligned} W'_n(-1) &= (\log(2) - \gamma) W_n(-1) - \int_0^\infty \log(x) J_0^n(x) dx, \\ W'_n(1) &= \int_0^\infty \frac{n}{x} J_0^{n-1}(x) J_1(x) (1 - \gamma - \log(2x)) dx. \end{aligned}$$

We may therefore obtain many identities by comparing the above equations to known values, for instance

$$3 \int_0^\infty \log(x) J_0^2(x) J_1(x) dx = \log(2) - \gamma - \frac{1}{\pi} \text{Cl} \left(\frac{\pi}{3} \right).$$

◇

In fact, the hypergeometric representation of W_3 and W_4 , (2.18) and (2.19) proven in Chapter 2, also make derivation of the derivatives of W_3 and W_4 possible.

Example 3.6.3 (Evaluation of $W_3'(0)$ and $W_4'(0)$). If we write (2.18) or (2.19) 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 (2.18) by appealing to the product rule, we get

$$W_3'(0) = \frac{1}{\pi} {}_3F_2 \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{1}{4} \right) = \frac{1}{\pi} \text{Cl} \left(\frac{\pi}{3} \right).$$

The last equality follows from setting $\theta = \pi/6$ in the identity

$$2 \sin(\theta) {}_3F_2 \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \sin^2 \theta \right) = \text{Cl}(2\theta) + 2\theta \log(2 \sin \theta), \quad (3.62)$$

Likewise, differentiating (2.19) gives

$$W_4'(0) = \frac{4}{\pi^2} {}_4F_3 \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1 \middle| 1 \right) = \sum_{n=0}^{\infty} \frac{1}{(2n+1)^3} = \frac{7\zeta(3)}{2\pi^2}, \quad (3.63)$$

thus verifying (3.59). ◇

Differentiating (2.18) at $s = 2$ leads to the evaluation

$${}_3F_2 \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{1}{4} \right) = \frac{27}{4} \left(\text{Cl} \left(\frac{\pi}{3} \right) - \frac{\sqrt{3}}{2} \right),$$

while from (2.19) at $s = 2$ we obtain

$$W_4'(2) = 3 + \frac{14\zeta(3) - 12}{\pi^2}. \quad (3.64)$$

Thus we have enough information to evaluate (3.53) (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.

The same technique yields

$$W_3''(0) = \frac{\pi^2}{12} + \frac{4 \log(2)}{\pi} \text{Cl} \left(\frac{\pi}{3} \right) - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\binom{2n}{n}}{4^{2n}} \frac{\sum_{k=0}^n \frac{1}{2k+1}}{(2n+1)^2}, \quad (3.65)$$

and, quite remarkably,

$$\begin{aligned} W_4''(0) &= \frac{\pi^2}{12} + \frac{7\zeta(3)\log(2)}{\pi^2} + \frac{4}{\pi^2} \sum_{n=0}^{\infty} \frac{H_n - 3H_{n+1/2}}{(2n+1)^3} \\ &= \frac{24\text{Li}_4\left(\frac{1}{2}\right) - 18\zeta(4) + 21\zeta(3)\log(2) - 6\zeta(2)\log^2(2) + \log^4(2)}{\pi^2}, \end{aligned} \quad (3.66)$$

where the very final evaluation is obtained from results in [58, §5] (more sums of this type are evaluated in Chapter 13). Here $\text{Li}_4(x)$ is the *polylogarithm* of order 4, while the continuation of H_n is given by $\gamma + \Psi(n+1)$ and Ψ is the *digamma* function (see (5.24)). So for non-negative integers n , we have $H_n = \sum_{k=1}^n 1/k$ 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 [55] and reprised in Chapter 9. In particular, this gives an evaluation of the sum on the right-hand side of (3.65).

Finally, the corresponding sum for $W_4''(2)$ may be split into a telescoping part and a part containing $W_4''(0)$. Therefore, it can also be written as a linear combination of the constants used in (3.66). In summary, we have all the pieces to evaluate (3.54), obtaining the answer $9\log(2)/(2\pi^2)$.

3.6.1. Relations with Mahler measures. For a (Laurent) polynomial $f(x_1, x_2, \dots, x_n)$, its *logarithmic Mahler measure*, see for instance [168], is defined as

$$\mu(f) = \int_0^1 \dots \int_0^1 \log |f(e^{2\pi i t_1}, \dots, e^{2\pi i t_n})| dt_1 \dots dt_n. \quad (3.67)$$

Recall that the s th moments of an n -step random walk are given by

$$W_n(s) = \int_0^1 \dots \int_0^1 \left| \sum_{k=1}^n e^{2\pi i t_k} \right|^s dt_1 \dots dt_n = \|x_1 + \dots + x_n\|_s^s$$

where $\|\cdot\|_p$ denotes the p -norm over the unit n -torus, and hence

$$W_n'(0) = \mu(x_1 + \dots + x_n) = \mu(1 + x_1 + \dots + x_{n-1}). \quad (3.68)$$

Thus the derivative evaluations in the previous sections are also Mahler measure evaluations. In particular, we rediscovered

$$W_3'(0) = \frac{1}{\pi} \text{Cl}\left(\frac{\pi}{3}\right) = \mu(1 + x_1 + x_2),$$

along with

$$W_4'(0) = \frac{7\zeta(3)}{2\pi^2} = \mu(1 + x_1 + x_2 + x_3)$$

which are both due to C. Smyth [168, (1.1) and (1.2)] with proofs first published in [60, Appendix 1].

With this connection realised, we find the following conjectural expressions put forth by Rodriguez-Villegas, mentioned in a different form in [93],

$$W_5'(0) \stackrel{?}{=} \left(\frac{15}{4\pi^2}\right)^{5/2} \int_0^\infty \{\eta^3(e^{-3t})\eta^3(e^{-5t}) + \eta^3(e^{-t})\eta^3(e^{-15t})\} t^3 dt, \quad (3.69)$$

$$W_6'(0) \stackrel{?}{=} \left(\frac{3}{\pi^2}\right)^3 \int_0^\infty \eta^2(e^{-t})\eta^2(e^{-2t})\eta^2(e^{-3t})\eta^2(e^{-6t}) t^4 dt, \quad (3.70)$$

where η was defined in (3.40). We have confirmed numerically that the evaluation of $W_5'(0)$ in (3.69) holds to 600 places, and that (3.70) holds to 80 places. Details of these somewhat arduous confirmations are given in [19].

Differentiating the series expansion for $W_n(s)$ obtained in Chapter 2 term by term, we obtain

$$W_n'(0) = \log(n) - \sum_{m=1}^{\infty} \frac{1}{2m} \sum_{k=0}^m \binom{m}{k} \frac{(-1)^k W_n(2k)}{n^{2k}}. \quad (3.71)$$

On the other hand, from [168] we find the strikingly similar

$$W_n'(0) = \frac{1}{2} \log(n) - \frac{\gamma}{2} - \sum_{m=2}^{\infty} \frac{1}{2m} \sum_{k=0}^m \binom{m}{k} \frac{(-1)^k W_n(2k)}{k! n^k}. \quad (3.72)$$

Finally, we note that $W_n(s)$ itself is a special case of *zeta Mahler measure* as introduced recently in [5]. We come back to Mahler measures in Chapters 8 and 9.

3.7. New results on W_n

In this section, we resolve a central case of Conjecture 1.1, among proving other identities. We heavily borrow results from [20].

From [20, equation (23)], we have for even $k > 0$,

$$W_3(k) = \frac{3^{k+3/2}}{\pi 2^k \Gamma(k/2 + 1)^2} \int_0^\infty t^{k+1} K_0(t)^2 I_0(t) dt, \quad (3.73)$$

where $I_0(t)$, $K_0(t)$ denote the *modified Bessel functions* of the first and second kinds, respectively.

Similarly, [20, (55)] states that for even $k > 0$,

$$W_4(k) = \frac{4^{k+2}}{\pi^2 \Gamma(k/2 + 1)^2} \int_0^\infty t^{k+1} K_0(t)^3 I_0(t) dt. \quad (3.74)$$

Equation (3.73) can be reduced to a closed form as a ${}_3F_2$, below (for instance using *Mathematica*). We are thus led to:

Theorem 3.9 (Single hypergeometric for $W_3(s)$). *For s not a negative integer less than -1 ,*

$$W_3(s) = \frac{3^{s+3/2} \Gamma(1 + s/2)^2}{2\pi \Gamma(s + 2)} {}_3F_2 \left(\begin{matrix} \frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2} \\ 1, \frac{s+3}{2} \end{matrix} \middle| \frac{1}{4} \right). \quad (3.75)$$

PROOF. It can be easily checked that both sides agree for $k = -1, 0, 1, 2$, and also satisfy the same recursion (using Zeilberger's algorithm). Therefore they agree for all integers $s > -2$. We shall now use Carlson's theorem, recorded as Theorem 1.3 in Chapter 1. Both sides of (3.75) are of exponential type, and standard estimate shows that the right-hand side is bounded by $e^{|y|\pi/2}$ on the imaginary axis. Therefore the conditions of Carlson's theorem are satisfied and the identity holds whenever the right-hand side converges. It also follows that (3.73) holds for all k with $\operatorname{Re} k > -2$. \square

Turning our attention to the negative integers, we have for integer $k \geq 0$:

$$W_3(-2k - 1) = \frac{4}{\pi^3} \left(\frac{2^k k!}{(2k)!} \right)^2 \int_0^\infty t^{2k} K_0(t)^3 dt, \quad (3.76)$$

because the two sides satisfy the same recursion [20, (8)], and agree when $k = 0, 1$ [20, (47) and (48)].

Remark 3.7.1. Equation (3.76) however does not hold when k is not an integer. Also, combining (3.76) and (3.73) for $W_3(-1)$, we deduce

$$\int_0^\infty K_0(t)^2 I_0(t) dt = \frac{2}{\sqrt{3}\pi} \int_0^\infty K_0(t)^3 dt = \frac{\pi^2}{2\sqrt{3}} \int_0^\infty J_0(t)^3 dt.$$

Integrals of $t^{2k} K_0(t)^3$ and $t^{2k+1} K_0(t)^3 I_0(t)$, among others, have been studied recently in a statistical mechanics context [156]. \diamond

From (3.76), we experimentally determined a single hypergeometric for $W_3(s)$ at negative odd integers:

Lemma 3.1. For $k \geq 0$ an integer,

$$W_3(-2k-1) = \frac{\sqrt{3} \binom{2k}{k}^2}{2^{4k+1} 3^{2k}} {}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ k+1, k+1 \end{matrix} \middle| \frac{1}{4} \right). \quad (3.77)$$

PROOF. It is easy to check that both sides agree at $k = 0$ and 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 is easily verified by *Maple*, or can be readily checked by Zeilberger's algorithm. A different proof is also illustrative: denote the right hand side of (3.77), with argument x instead of $1/4$, by $F_k(x)$. In Chapter 14, a general method is given which allows us to write $F_{k+1}(x)$ as a differential operator of $F_k(x)$. Therefore, the recursion satisfied by the W_3 side gives a differential expression for F_k , which can be simplified using the third order differential equation also satisfied by F_k . In the simplified expression, the factor $1 - 4x$ emerges, so it equals 0 identically when $x = 1/4$. \square

The integral in (3.76) shows that $W_3(-2k-1)$ decays to 0 rapidly – very roughly like 9^{-k} as $k \rightarrow \infty$ – and so is never 0 when k is an integer.

To show that (3.74) holds for more general k required more work. Using Nicholson's integral representation in [195],

$$I_0(t)K_0(t) = \frac{2}{\pi} \int_0^{\pi/2} K_0(2t \sin a) da,$$

the integral in (3.74) simplifies to

$$\frac{2}{\pi} \int_0^{\pi/2} \int_0^\infty t^{k+1} K_0(t)^2 K_0(2t \sin a) dt da. \quad (3.78)$$

The inner integral in (3.78) 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, via (2.29), 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 function, so the outer integral in (3.78) transforms to

$$\frac{\sqrt{\pi}}{16} \int_0^1 t^{-\frac{k+3}{2}} (1-t)^{-\frac{1}{2}} G_{3,3}^{2,3} \left(\begin{matrix} 1, 1, 1 \\ \frac{3}{2}, \frac{3}{2}, \frac{1}{2} \end{matrix} \middle| t \right) dt. \quad (3.79)$$

We can resolve this integral by applying the Euler-type integral

$$\int_0^1 t^{-a}(1-t)^{a-b-1} G_{p,q}^{m,n} \left(\begin{matrix} \mathbf{c} \\ \mathbf{d} \end{matrix} \middle| zt \right) dt = \Gamma(a-b) G_{p+1,q+1}^{m,n+1} \left(\begin{matrix} a, \mathbf{c} \\ \mathbf{d}, b \end{matrix} \middle| z \right). \quad (3.80)$$

Indeed, when $k = -1$, the application of (3.80) recovers the Meijer G representation of $W_4(-1)$ in Chapter 2; that is, (3.74) 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 [153], turning it into the triple integral (up to a constant factor)

$$\int_0^1 \int_0^1 \int_0^1 \sqrt{\frac{x(1-x)z}{y(1-y)(1-z)(1-x(1-yz))^3}} dx dy dz.$$

We can reduce the triple integral to a single integral,

$$\int_0^1 \frac{8E'(t)((1+t^2)K'(t) - 2E'(t))}{(1-t^2)^2} dt.$$

Now applying the change of variable $t \mapsto (1-t)/(1+t)$, followed by quadratic transformations for K and E [46], we finally get the expression

$$\int_0^1 \frac{4(1+t)}{t^2} E \left(\frac{2\sqrt{t}}{1+t} \right) (K(t) - E(t)) dt, \quad (3.81)$$

which is, indeed, the correct constant multiple times the expression for $W_4(1)$ in (2.49).

(In fact, in view of our results and techniques presented in Chapters 6 and 7, we can simplify the integral (3.81) directly. Cleaning up the first E term using a quadratic transform, we then integrate $\frac{1-t^2}{t}(5E(t)K(t) - 2K(t)^2 - 3E(t)^2)$ by parts and add the result to our integral in order to clear the $1/t^2$ in the denominator. The expression produced is a linear combination of the moments of $E(t)^2$, $K(t)^2$ and $E(t)K(t)$, which can be simplified to (2.34).)

We finally observe that both sides of (3.74) satisfy the same recursion [20, (9)], hence they agree for $k = 0, 1, 2, \dots$. Carlson's theorem applies since the growth on the imaginary axis is the same as for (3.73), so we have proven:

Lemma 3.2. *Equation (3.74) holds for all k with $\operatorname{Re} k > -2$.*

Theorem 3.10 (Alternative Meijer G representation for $W_4(s)$). *For all s ,*

$$W_4(s) = \frac{2^{2s+1}}{\pi^2 \Gamma(\frac{1}{2}(s+2))^2} G_{4,4}^{2,4} \left(\begin{matrix} 1, 1, 1, \frac{s+3}{2} \\ \frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2}, \frac{1}{2} \end{matrix} \middle| 1 \right). \quad (3.82)$$

PROOF. Apply (3.80) to (3.79) for general k , and equality holds by Lemma 3.2. \square

Note that Lemma 3.2 combined with the formula for $W_4(-1)$ in Chapter 2 gives the Bessel identity

$$\frac{4}{\pi^3} \int_0^\infty K_0(t)^3 I_0(t) dt = \int_0^\infty J_0(t)^4 dt. \quad (3.83)$$

Armed with the knowledge of Lemma 3.2, we may now resolve a very special but central case (corresponding to $n = 2$) of Conjecture 1.1.

Theorem 3.11. *For integer s ,*

$$W_4(s) = \sum_{j=0}^{\infty} \binom{s/2}{j}^2 W_3(s-2j). \quad (3.84)$$

PROOF. In Chapter 1 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 (3.84) is

$$\sum_{j=0}^{\infty} \binom{-1/2}{j}^2 W_3(-1-2j) = \sum_{j=0}^{\infty} \frac{2^{2-2j}}{\pi^3 j!^2} \int_0^\infty t^{2j} K_0(t)^3 dt$$

upon using (3.76). After interchanging summation and integration (which is justified as all terms are positive), this reduces to

$$\frac{4}{\pi^3} \int_0^\infty K_0(t)^3 I_0(t) dt,$$

which is the value for $W_4(-1)$ by Lemma 3.2.

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 (3.84) at $s = -3$, and interchanging summation and integration as before, we obtain

$$\sum_{j=0}^{\infty} \binom{-3/2}{j}^2 W_3(-3-2j) = \frac{4}{\pi^3} \int_0^\infty t^2 K_0(t)^3 I_0(t) dt = \frac{1}{64} W_4(1) = W_4(-3).$$

Therefore (3.84) holds when $s = -1, -3$, and thus holds for all integer s . \square

CHAPTER 4

More Results on Uniform Random Walks

ABSTRACT. In this chapter we include a number of results on random walks which do not fit into the context of the first three chapters. In particular, we investigate uniform random walks with different step sizes, or confined to a limited number of directions, or lifted to higher dimensions.

4.1. Elementary derivations of p_2 and p_3

The probability density p_2 (equation (3.1), Chapter 3) may be derived from completely elementary considerations. Without loss of generality, we start from the origin and let the first step land on the point $(0, 1)$. For the second step to land inside the circle with radius r centred at the origin, it must be contained between the two tangents to the circle from $(0, 1)$. Using basic trigonometry, the angle between the two tangents is $4\text{asin}(r/2)$, therefore the cumulative distribution $P_2(r) = 4\text{asin}(r/2)/(2\pi)$. Taking the derivative with respect to r recovers

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

Example 4.1.1. We can achieve a bit more with the same argument. Let $p_2^a(r)$ denote the probability density of a 2-step walk where the step lengths are 1 and a (without loss of generality, in this order). We consider the angle θ between these two steps, such that the walker ends up in a circle of radius r . The cosine rule gives $|\theta| \leq \text{acos}\left(\frac{a^2+1-r^2}{2a}\right)$. Consequently,

$$p_2^a(r) = \frac{2r}{\pi\sqrt{4a^2 - (1+a^2-r^2)^2}}, \quad |a-1| \leq r \leq a+1. \quad (4.1)$$

The general expression for the s th moment of the distance from the origin is

$$\frac{1}{\pi} \int_0^\pi (a^2 + 1 + 2a \cos(t))^{s/2} dt = (1+a)^s {}_2F_1\left(\begin{matrix} -\frac{s}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| \frac{4a}{(1+a)^2}\right), \quad (4.2)$$

since after a change of variable, the left hand side integral is of Euler-type for a ${}_2F_1$ [11], i. e. it is of the form

$$\int_0^1 x^{b-1}(1-x)^{c-b-1}(1-zx)^{-a} dx = \frac{\Gamma(b)\Gamma(c-b)}{\Gamma(c)} {}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix} \middle| z\right). \quad (4.3)$$

In particular, the (-1) st, 1st and 2nd moments are, respectively, $\frac{2}{\pi(a+1)}K\left(\frac{2\sqrt{a}}{a+1}\right)$, $\frac{2(a+1)}{\pi}E\left(\frac{2\sqrt{a}}{a+1}\right)$ and $a^2 + 1$. \diamond

We now give an elementary derivation for the density p_3 . Again, let the first step fall on $(0, 1)$, and let the second step form an angle t with the positive x -axis (by symmetry let $t \geq 0$); it therefore lands on the point $(1 + \cos(t), \sin(t))$. Now consider a circle of radius $r > 1$; the $r \leq 1$ case is very similar. The third step needs to be confined within this circle, so it must be contained between the two blue radii shown on the right of Figure 1. The angle s between these two radii can be found using trigonometry, using the coordinates of the intersections between the circles $x^2 + y^2 = r^2$ and $(x - 1 - \cos(t))^2 + (y - \sin(t))^2 = 1$.

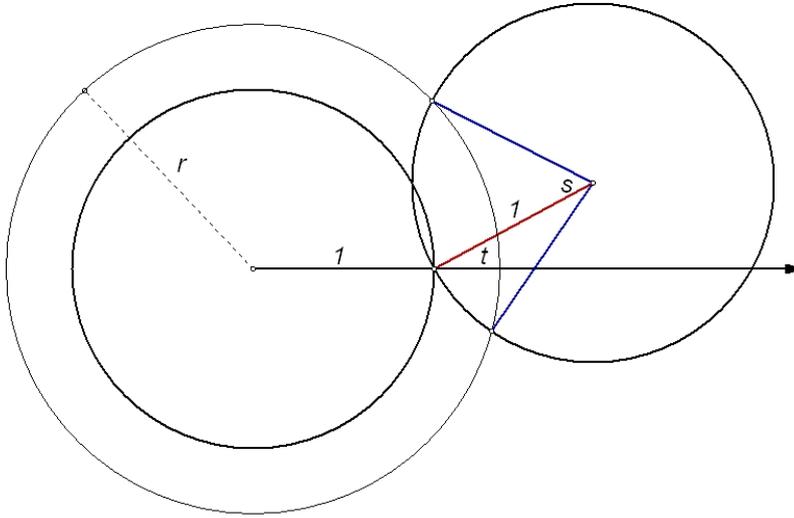


FIGURE 1. Elementary derivation of p_3 . The origin is on the left; lengths and angles are marked.

The two circles do not always intersect; for $r > 1$, they intersect when $0 \leq t \leq t_1$, where $t_1 = \arccos\left(\frac{1}{2}(r^2 - 2r - 1)\right)$. For t in this domain, we can calculate that

$$4 \sin \frac{s}{2} = \sqrt{8r^2 - 8 \cos(t) - \frac{2(r^2 - 1)^2}{1 + \cos(t)}}.$$

Therefore, when $r > 1$, we have

$$p_3(r) = \frac{1}{2\pi^2} \frac{d}{dr} \int_0^{t_1} s \, dt. \quad (4.4)$$

After a few trigonometric and linear changes of variables, we simplify (4.4) down to

$$p_3(r) = \frac{1}{2\pi^2} \int_0^1 \left[t(1-t) \left(\frac{(3-r)(1+r)}{4r} - t \right) \left(\frac{(r-1)^2}{4r} + t \right) \right]^{-1/2} dt.$$

This can be computed using the help of

$$\int_0^1 \frac{dt}{\sqrt{t(1-t)(a-t)(b-t)}} = \frac{2}{\sqrt{a(b-1)}} K \left(\sqrt{\frac{b-a}{a(b-1)}} \right). \quad (4.5)$$

When $r \leq 1$, the only difference we make to the above derivation is that the two circles intersect when $t_0 \leq t \leq t_1$, where $t_0 = \arccos(\frac{1}{2}(r^2 + 2r - 1))$, and we proceed similarly for the rest of the calculation. We thus obtain

$$p_3(r) = \begin{cases} \frac{\sqrt{r}}{\pi^2} K \left(\sqrt{\frac{(3-r)(1+r)^3}{16r}} \right) & \text{if } r > 1 \\ \frac{4r}{\pi^2 \sqrt{(3-r)(1+r)^3}} K \left(\sqrt{\frac{16r}{(3-r)(1+r)^3}} \right) & \text{if } r \leq 1. \end{cases}$$

Relating the two cases using Jacobi's imaginary transformation [46], the formulas for p_3 obtained above agree with equation (3.2).

Remark 4.1.1. We remark that (4.5) itself can be proven by the change of variable $x = (b-1)t/(b-t)$ – that is, a Möbius transformation fixing two of the singularities in the integrand and sending another to infinity – this makes the denominators into the square root of a cubic. Evaluations like this are not flukes, but merely reflect the fact that the underlying algebraic curves have genus one (see e. g. [178]). \diamond

4.2. Three-step walk with different step lengths

We now look at the 3-step walk in which the step sizes are different. Without loss of generality, we can let the first step length be 1, the second be a , and the third be b . Then, mirroring the integral in (1.1), the average distance from the origin is

$$\int_0^1 \int_0^1 \sqrt{(1 + a \cos(2\pi s) + b \cos(2\pi t))^2 + (a \sin(2\pi s) + b \sin(2\pi t))^2} \, ds dt.$$

We follow closely the analysis for $W_3(1)$ in Chapter 1; thus we first attempt to simplify the trigonometric expression in the integrand. It turns out that a clean

reduction is only possible when (without loss of generality) $b = 1$, so in this case, denoting the average distance from the origin by D_a , we have

$$D_a = \int_0^1 \int_0^1 \sqrt{2 + a^2 + 2 \cos(2\pi t) + 4a \cos(\pi(2s - t)) \cos(\pi t)} \, ds dt. \quad (4.6)$$

From the periodicity of the integral in (4.6), we make a change of variable and obtain

$$D_a = \int_0^1 \int_0^1 \sqrt{2 + a^2 + 2 \cos(2\pi t) + 4a \cos(2\pi s) \cos(\pi t)} \, ds dt. \quad (4.7)$$

Since

$$\int_0^\pi \sqrt{A + B \cos(t)} \, dt = 2\sqrt{A + B} E\left(\sqrt{\frac{2B}{A + B}}\right), \quad (4.8)$$

we can evaluate the t integral in (4.7); after a trigonometric change of variable, we get

$$D_a = \frac{4a^2}{\pi^2} \int_0^{2/a} \frac{1+x}{\sqrt{4-a^2x^2}} E\left(\frac{2\sqrt{x}}{1+x}\right) dx.$$

As was done for the analysis for $W_3(1)$, we apply Jacobi's imaginary transformations (1.35) to the E term, which leads to

$$D_a = \frac{4a^2}{\pi^2} \operatorname{Re} \int_0^{2/a} \frac{2E(x) - (1-x^2)K(x)}{\sqrt{4-a^2x^2}} dx.$$

Next, we expand E and K as series, interchange the order of summation and integration and appeal to analytic continuation. This gives the next theorem:

Theorem 4.1. *With $f(a) := \sqrt{(1 - \sqrt{1 - 4/a^2})/2}$, we have*

$$D_a = \frac{4a}{\pi} \left(6E(f(a))^2 - 4(2 - f(a)^2)E(f(a))K(f(a)) + (3 - 2f(a)^2)K(f(a))^2 \right). \quad (4.9)$$

In particular, $f(2) = 1/\sqrt{2}$ is the first singular value, so the elliptic integrals can be easily evaluated, producing the following closed form:

Corollary 4.1. *In a 3-step uniform random walk, the average distance from the origin when the step sizes are 1, 1 and 2 is*

$$D_2 = \frac{48\pi}{\Gamma^4(\frac{1}{4})} + \frac{\Gamma^4(\frac{1}{4})}{4\pi^3}. \quad (4.10)$$

Note that we may work out the (-1) st moment analogously, using instead the formula

$$\int_0^\pi \frac{dt}{\sqrt{A + B \cos(t)}} = \frac{2}{\sqrt{A + B}} K\left(\sqrt{\frac{2B}{A + B}}\right), \quad (4.11)$$

and the imaginary transformation

$$K(1/k) = k(K(k) + iK'(k)).$$

It follows that the (-1) st moment of a 3-step walk with step sizes 1, 1 and 2 is $\Gamma^4(1/4)/(4\pi^3)$.

4.3. Higher dimensions

We start with a motivating example.

Example 4.3.1. The geometric argument from which we found p_2 in Section 4.1 generalises to give a very simple expression for the 2-step probability density of a uniform random walk in three dimensions, which we denote by $p_2^{(3)}$. Here, instead of seeking the arc-length subtended by the half-angle $t = 2\text{asin}(r/2)$ from the origin, we need to find the surface area of a spherical cap subtended by a cone with the same half-angle. The surface area of a (unit-)spherical cap is conveniently $2\pi h$, where h is the height of the cap. Since in this case $h = 1 - \cos(t)$, we have the very elegant formula

$$p_2^{(3)} = \frac{d}{dr} \frac{2\pi(1 - \cos(2\text{asin}\frac{r}{2}))}{4\pi} = \frac{r}{2}. \quad (4.12)$$

From this, we easily obtain that the s th moment of the distance for the 2-step walk in 3D is $2^{s+1}/(s+2)$. The 1st moment, $4/3$, can also be found independently as an elementary single integral, by fixing the first step and then using spherical coordinates and the Jacobian. \diamond

We will now compute two general results using elementary multi-dimensional integrals. The first result is the s th moment (of the distance from the origin) of the 2-step walk in any dimension d , denoted by $W_2^{(d)}(s)$. The second result is the 2nd moment of the n -step walk in any dimension d , $W_n^{(d)}(2)$. We again begin with simpler examples.

Example 4.3.2. We first show that in 3D, the 2nd moment for the n -step walk is n . Indeed, using spherical coordinates, we have

$$\begin{aligned} W_n^{(3)}(2) &= \frac{1}{(4\pi)^n} \int_{t_1=0}^{\pi} \cdots \int_{t_n=0}^{\pi} \int_{s_1=0}^{2\pi} \cdots \int_{s_n=0}^{2\pi} dt_1 \cdots dt_n ds_1 \cdots ds_n \sin(t_1) \cdots \sin(t_n) \\ &\quad \times \left[\left(\sum_{i=1}^n \sin(t_i) \cos(s_i) \right)^2 + \left(\sum_{i=1}^n \sin(t_i) \sin(s_i) \right)^2 + \left(\sum_{i=1}^n \cos(t_i) \right)^2 \right], \end{aligned}$$

where the first line of the integrand contains the Jacobian. By symmetry (since we can rotate the coordinate system), the second line of the integrand may be replaced by $3(\sum_{i=1}^n \cos(t_i))^2$. We expand out the new integrand and note that only the $\cos^2(t_i)$ terms do not vanish; now the claimed evaluation follows by elementary integration. \diamond

A more involved computation, similar to Example 4.3.2, leads to:

Theorem 4.2. *The 2nd moment of the distance from the origin for the n -step walk in d -dimensions is n .*

PROOF. We proceed as we did for the 3D case. For d -dimensions we need the hyper-spherical coordinates, the expression for the Jacobian, the surface area of the d -dimensional unit sphere, and we again appeal to symmetry. Gathering everything together, we have

$$W_n^{(d)}(2) = d \left(\frac{\Gamma(d/2 + 1)}{d \pi^{d/2}} \right)^n \int_C \left(\sum_{i=1}^n \cos(t_{1i}) \right)^2 \prod_{j=1}^{d-2} \prod_{k=1}^n \sin^{d-1-j}(t_{jk}),$$

where \int_C involves integrating with respect to the variables t_{jk} where $1 \leq j \leq d-2$ and $1 \leq k \leq n$; the interval of integration is from 0 to 2π for $t_{(d-1)k}$, and from 0 to π for all other t_{jk} .

As in the 3D case, only the $\cos^2(t_{1i})$ terms survive the expansion, and we have, after simplification,

$$W_n^{(d)}(2) = d \left(\frac{\Gamma(d/2 + 1)}{d \pi^{d/2}} \right)^n (2\pi)^n n \frac{\int_0^\pi \cos^2(t) \sin^{d-2}(t) dt}{\int_0^\pi \sin^{d-2}(t) dt} \left(\prod_{j=1}^{d-2} \int_0^\pi \sin^j(r) dr \right)^n.$$

All the integrals on the right hand side are beta integrals (see equation (5.21)), and as such evaluate in terms of Gamma functions. The resulting product telescopes, and ultimately simplifies to n . \square

Example 4.3.3. We now find the s th moment of a 2-step walk in 4D. It is not hard to write down the integral,

$$W_2^{(4)}(s) = \frac{1}{2\pi^2} \int_0^{2\pi} \int_0^\pi \int_0^\pi dt ds dr \sin^2(t) \sin(s) \times \left[\sqrt{(\cos t + 1)^2 + (\sin t \cos s)^2 + (\sin t \sin s \cos r)^2 + (\sin t \sin s \sin r)^2} \right]^s.$$

The radical in the integrand simplifies to $2 \cos(t/2)$, and therefore we end up with a beta integral, with the evaluation

$$W_2^{(4)}(s) = \frac{2^{s+2} \Gamma(\frac{3+s}{2})}{\sqrt{\pi} \Gamma(3 + \frac{s}{2})}. \quad (4.13)$$

As expected, the 2nd moment is 2; more interestingly, the 1st moment (average) is $\frac{64}{15\pi}$. \diamond

We may generalise the result Example 4.3.3 in the following theorem:

Theorem 4.3. *The s th moment of the distance from the origin for the 2-step walk in d -dimensions is*

$$W_2^{(d)}(s) = \frac{2^{d+s-2} \Gamma(\frac{d}{2}) \Gamma(\frac{d+s-1}{2})}{\sqrt{\pi} \Gamma(d + \frac{s}{2} - 1)}. \quad (4.14)$$

PROOF. In hyper-spherical coordinates, fix the first step in an axis direction such that the second step only depends on the angle t_1 , so the distance from the origin may be modeled by $2 \cos(t_1/2)$ (as in the 4D case). Inserting the volume for the n -dimensional unit sphere and the Jacobian, we have

$$\begin{aligned} W_2^{(d)}(s) &= \frac{\Gamma(\frac{d}{2} + 1)}{d \pi^{d/2}} \int_0^{2\pi} \int_0^\pi \cdots \int_0^\pi \sin^{d-2}(t_1) \sin^{d-3}(t_2) \cdots \sin(t_{d-2}) \\ &\quad \times \left(2 \cos \frac{t_1}{2}\right)^s dt_1 \cdots dt_{d-1}. \end{aligned}$$

This factors into a product of beta integrals; the product also telescopes, and simplifies to the claimed evaluation. \square

Since the probability density is the inverse Mellin transform of the moments (c.f. Chapter 3, Section 2), by residue calculus we immediately have the following result:

Corollary 4.2. *The probability density for the 2-step walk in d -dimensions is*

$$p_2^{(d)}(r) = \frac{r^{d-2}}{\sqrt{\pi} 2^{d-3}} \frac{\Gamma(\frac{d}{2})}{\Gamma(\frac{d-1}{2})} (4 - r^2)^{(d-3)/2}. \quad (4.15)$$

This recaptures the formula (4.12) for $p_2^{(3)}(r)$ and also gives $p_2^{(4)}(r) = r^2 \sqrt{4 - r^2} / \pi$.

4.3.1. A closer look at three dimensions. Watson [195] records a general formula for the cumulative distribution for the n -step walk in d -dimensions:

$$\int_0^r p_n^{(d)}(s) ds = \Gamma\left(\frac{d}{2}\right)^{n-1} r^{d/2} \int_0^\infty \left(\frac{2}{t}\right)^{(n-1)(d/2-1)} J_{d/2}(rt) J_{d/2-1}(t)^n dt. \quad (4.16)$$

Since the Bessel function is elementary at half integer orders, (4.16) allows us to analyse the probability density in odd-dimensions.

Example 4.3.4. For instance, the n -step density in 3D is given by the integral

$$\frac{2}{\pi} \int_0^\infty \frac{r \sin^n(t) \sin(rt)}{t^{n-1}} dt, \quad (4.17)$$

and since the (indefinite) integral evaluates in terms of the sine integral, we find for instance

$$p_3^{(3)}(r) = \begin{cases} \frac{r^2}{2} & \text{if } r \in [0, 1] \\ \frac{r(3-r)}{4} & \text{if } r \in [1, 3], \end{cases} \quad (4.18)$$

and therefore $W_3^{(3)}(s) = \frac{3(3^{s+2}-1)}{4(s+2)(s+3)}$, in particular the average distance is $13/8$. Note the expression for $W_3^{(3)}(s)$ has an analytic continuation to the whole complex plane with a simple pole at -3 . Similarly,

$$p_4^{(3)}(r) = \begin{cases} \frac{r^2(8-3r)}{16} & \text{if } r \in [0, 2] \\ \frac{r(4-r)^2}{16} & \text{if } r \in [2, 4], \end{cases} \quad (4.19)$$

and therefore $W_4^{(3)}(s) = \frac{2^{s+3}(2^{s+2}-1)}{(s+2)(s+3)(s+4)}$, in particular the average distance is $28/15$. The expression for $W_4^{(3)}(s)$ is meromorphic with simple poles at -3 and -4 . \diamond

Indeed, we have:

Theorem 4.4. *The probability density for the distance from the origin for the n -step walk in 3D is given by the following piecewise-polynomial,*

$$p_n^{(3)}(r) = \frac{r(n-2i-r)^{n-2}}{2^n(n-2)!} \sum_{i=0}^n \binom{n}{i} (-1)^i \operatorname{sgn}(n-2i-r), \quad (4.20)$$

where $\operatorname{sgn}(x)$ denotes the sign of x .

PROOF. Using the formula

$$\sin^n t = \begin{cases} \sum_{i=0}^n \binom{n}{i} (-1)^{i+n/2} 2^{-n} \cos((n-2i)t) & \text{if } n \text{ is even} \\ \sum_{i=0}^n \binom{n}{i} (-1)^{i+(n-1)/2} 2^{-n} \sin((n-2i)t) & \text{if } n \text{ is odd,} \end{cases} \quad (4.21)$$

we find after some algebra that

$$\frac{d^{n-2}}{dt^{n-2}} \sin^n(t) \sin(rt) = \sum_{i=0}^n \binom{n}{i} (-1)^i (n-2i-r)^{n-2} 2^{-n} \sin((n-2i-r)t). \quad (4.22)$$

We also need the fact that

$$\int_0^\infty \frac{\sin(rt)}{t} dt = \frac{\pi}{2} \operatorname{sgn}(r). \quad (4.23)$$

Now, equation (4.20) follows from integrating (4.17) by parts $(n-2)$ times, and simplifying the result using (4.22) and (4.23). \square

We may use equation (4.20) to find (the analytic continuations of) the moments in 3D, which are elementary expressions. On the other hand, we may use elementarily derived results to evaluate non-trivial integrals which are special cases of (4.16).

For example, Theorem 4.2 combined with (4.16) produces

$$\int_0^\infty \int_0^n r^{d/2+2} t^{n-d(n-1)/2} J_{d/2-1}(t)^n J_{d/2-1}(rt) dr dt = \frac{n 2^{(d/2-1)(1-n)}}{\Gamma(\frac{d}{2})^{n-1}}. \quad (4.24)$$

Similarly, Theorem 4.3 combined with (4.16) gives the evaluation

$$\int_0^\infty \int_0^2 r^{d/2+s} t^{2-d/2} J_{d/2-1}(t)^2 J_{d/2-1}(rt) dr dt = \frac{2^{d/2+s-1} \Gamma(\frac{d+s-1}{2})}{\sqrt{\pi} \Gamma(d + \frac{s}{2} - 1)}. \quad (4.25)$$

And finally, with (4.1), we obtain

$$\int_0^\infty t J_0(t) J_0(at) J_0(rt) dt = \frac{2}{\pi \sqrt{4a^2 - (1+a^2-r^2)^2}}.$$

Remark 4.3.1 (Probability of return). We can also use (4.16) to find the probability of returning to the unit sphere after n steps in 3 dimensions. Indeed, putting $r = 1$ and simplifying the resulting integral by parts, the required probability is

$$\frac{2}{(n+1)\pi} \int_0^\infty \operatorname{sinc}(t)^{n+1} dt, \quad (4.26)$$

where $\operatorname{sinc}(t) = \sin(t)/t$. A treatment of the sinc integrals (4.26) has been given by many authors (see for instance [38]); expressions in terms of finite sums are known, for we may apply (4.21) and integration by parts to deduce

$$\int_0^\infty \operatorname{sinc}(t)^n dt = \frac{\pi}{2^n (n-1)!} \sum_{i=0}^{\lfloor \frac{n}{2} \rfloor} \binom{n}{i} (-1)^i (n-2i)^{n-1}. \quad (4.27)$$

When n is even, the right hand sum conveniently simplifies:

$$\int_0^\infty \operatorname{sinc}(t)^{2n} dt = \frac{\pi}{2(2n-1)!} \left\langle \begin{matrix} 2n-1 \\ n-1 \end{matrix} \right\rangle.$$

Here $\langle \binom{n}{k} \rangle$ is an *Eulerian numbers*, i. e. the number of permutations of n elements that have exactly k ascending runs [197, Ch. 1].

For $n = 2, 3, \dots$, the probabilities of returning to the unit sphere are given by

$$\frac{1}{4}, \frac{1}{6}, \frac{23}{192}, \frac{11}{120}, \frac{841}{11520}, \dots$$

where the first value ($1/4$) follows also by simple geometric considerations. Asymptotically, the probability of returning after n steps is roughly $\sqrt{\frac{6}{\pi(n+1)^3}}$ (see for instance [147], or use (4.28) below). \diamond

Example 4.3.5 (Asymptotics). By the *central limit theorem* (see also the next section) and the Mellin transform, it is not hard to find the asymptotic behaviour of the 3D walk for large n :

$$p_n^{(3)}(r) \approx 3\sqrt{\frac{6}{\pi}} n^{-\frac{3}{2}} r^2 e^{-\frac{3r^2}{2n}}, \quad W_n^{(3)}(s) \approx \frac{2}{\sqrt{\pi}} \left(\frac{2n}{3}\right)^{\frac{s}{2}} \Gamma\left(\frac{s+3}{2}\right). \quad (4.28)$$

In particular, the average distance from the origin after n steps is around $\sqrt{\frac{8n}{3\pi}}$.

For the uniform random walk on the *plane*, we may obtain better approximations of p_n than Rayleigh's $\frac{2x}{n} e^{-x^2/n}$ for large n . We follow Pearson's approach in [158], starting from writing Klyuyver's expression (3.5) as

$$p_n(x) = \int_0^\infty xt J_0(xt) (J_0(t) e^{t^2/4})^n e^{-nt^2/4} dt. \quad (4.29)$$

We expand out the parenthesised term as a series around $t = 0$. Truncating the series after k terms (let us call this truncation $S_k(t)$) gives a good approximation for $(J_0(t) e^{t^2/4})^n$ for small t , while for large t the $e^{-nt^2/4}$ factor compensates. Even for $S_2(t)$ (the partial expansion being $1 - nt^4/64$), we obtain the better approximation

$$p_n(x) \approx x e^{-\frac{x^2}{n}} \left(\frac{4n^3 - 2n^2 + 4nx^2 - x^4}{2n^4} \right). \quad (4.30)$$

This gives a more refined approximation to the mean $W_n(1)$ ($\sqrt{n\pi}/2 + \sqrt{\pi/n}/32$), and for the standard deviation ($\sqrt{n(1 - \pi/4) - \pi/32}$); compare with Remark 1.2.2.

Because of the connection (3.68) between $W'_n(0)$ and Mahler measures, we can use Pearson's idea to give an asymptotic expansion for the measure $\mu(1 + x_1 + \dots + x_{n-1})$ by computing the integral

$$\int_0^n \int_0^\infty S_k(t) e^{-nt^2/4} J_0(xt) xt \log(x) dt dx. \quad (4.31)$$

The double integral may be evaluated in closed form, thanks to the presence of the exponential. We take the answer of (4.31) and discard all terms that decay exponentially. For instance, using $S_3(t)$, we have

$$\mu(1 + x_1 + \cdots + x_{n-1}) \sim \frac{\log n}{2} - \frac{\gamma}{2} + \frac{1}{8n} + \frac{5}{288n^2} - \frac{1}{192n^3} + O(n^{-4}).$$

Unfortunately, the approximation is not great; for S_5 , we get only 6 digits of agreement for $n = 20$. ◇

4.4. Limiting the number of directions

In this section, we briefly comment on some asymptotic similarities between the two dimensional uniform random walk and the random walk with a limited number of directions. For instance, when we limit the walk to the four cardinal directions, then we end up with a walk on a square *lattice* [118].

Example 4.4.1. In the square lattice case, it is a simple combinatorial exercise to find the probability of ending up at coordinate (u, v) after n steps. Therefore, we may look quantitatively at the moments of the distance from the origin, which we call $Wl_n(s)$. Indeed, $Wl_n(2)$, being a double sum, may be evaluated, albeit tediously, by using contiguous versions of Dixon's identity (see Chapter 14). It transpires that $Wl_n(2)$ is exactly n , which equals the 2nd moment of a uniform random walk.

The 4th and the 6th moments are more unwieldy, and to evaluate them the multiple-Zeilberger algorithm [202] is the method of choice. In each case, perhaps unexpectedly, an order 1 recurrence is produced. Solving the recurrences, we have the results

$$Wl_n(4) = W_n(4), \quad Wl_n(6) = W_n(6).$$

However, agreement does *not* continue beyond this point, since $Wl_2(2s) = (4^s + 2^{s+1})/4$ and $W_2(2s) = \binom{2s}{s}$; therefore the 8th and higher even moments for these two walks are different. This phenomenon is more general: numerical evidence suggests that for the walk with k possible, evenly spread directions, the 0th, 2nd, 4th, \dots $(2k-2)$ th moments, and only these, agree with the corresponding moments of W_n . ◇

In a recent paper [14], the asymptotic behaviour of a random walk restricted to k directions (being the vertices of a regular k -gon) is considered. Applying the multivariate central limit theorem and using some trigonometric identities, it is shown that when $k > 2$, the resulting covariance matrix does not depend on k , and hence in the limit $k \rightarrow \infty$ we recover the uniform random walk. It follows that the asymptotic behaviour of the s th moment of the distance of an n -step walk (for any $k > 2$) is

$$E[\chi_2^s] \left(\frac{n}{2}\right)^{s/2},$$

where $E[\chi_2^s]$ denotes the expectation of the s th power of the χ distribution with 2 degrees of freedom. It follows by a standard change of variable and integration that asymptotically this is $n^{s/2}\Gamma(s/2+1)$, in agreement with a result obtained in Chapter 1. In particular, this shows that the average distance from the origin, regardless of the restriction on the number of directions, behaves like $W_n(1)$ when n is large.

The remaining case not covered by the asymptotics above is when $k = 2$ (the 1D lattice). In this case, unsurprisingly the asymptotic behaviour of the s th moment is $n^{s/2}$ times the expectation of the s th power of the half-normal distribution (that is, the normal distribution ‘folded’ around the mean at 0). This comes out to be

$$\frac{(2n)^{s/2} \Gamma(\frac{1+s}{2})}{\sqrt{\pi}},$$

and therefore, we recover the asymptotic distance from the origin, $\sqrt{2n/\pi}$.

Remark 4.4.1. We wrap up our foray into random walks by showing that when $s = 2$, the asymptotic behaviour of the distance from the origin, n , found above agrees with the exact result of the 2nd moment. This can be proven since the exact expression for the 2nd moment, when the walk is confined to k directions, is

$$\frac{1}{k^n} \sum_{t_i=1}^k \left(\cos \frac{2\pi t_1}{k} + \cos \frac{2\pi t_2}{k} + \cdots + \cos \frac{2\pi t_n}{k} \right)^2 + \left(\sin \frac{2\pi t_1}{k} + \sin \frac{2\pi t_2}{k} + \cdots + \sin \frac{2\pi t_n}{k} \right)^2.$$

We expand the brackets and observe that all the cross terms disappear in the summation. We then collect the $\cos^2(t) + \sin^2(t)$ terms and the answer n follows. \diamond

Moments of Elliptic Integrals and Catalan's Constant

ABSTRACT. We investigate the moments of Ramanujan's alternative elliptic integrals and of related hypergeometric functions. Along the way we are able to give some surprising closed forms for Catalan-related constants and various hypergeometric identities.

5.1. Introduction and background

As in [46, pp. 178–179], for $0 \leq s < 1/2$ and $0 \leq k \leq 1$, define the generalised elliptic integrals by

$$K^s(k) := \frac{\pi}{2} {}_2F_1\left(\begin{matrix} \frac{1}{2} - s, \frac{1}{2} + s \\ 1 \end{matrix} \middle| k^2\right), \quad (5.1)$$

$$E^s(k) := \frac{\pi}{2} {}_2F_1\left(\begin{matrix} -\frac{1}{2} - s, \frac{1}{2} + s \\ 1 \end{matrix} \middle| k^2\right). \quad (5.2)$$

We use the standard notation for hypergeometric functions, e. g.

$${}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix} \middle| z\right) := \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{z^n}{n!}$$

and its analytic continuation. One of the key early results, due to Gauss (1812), is the closed form

$${}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix} \middle| 1\right) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \quad (5.3)$$

when $\operatorname{Re}(c-a-b) > 0$.

We are interested in the *moments* given by

$$K_n = K_{n,s} := \int_0^1 k^n K^s(k) \, dk, \quad E_n = E_{n,s} := \int_0^1 k^n E^s(k) \, dk. \quad (5.4)$$

for both integer and real values of n . We immediately note that $K^s = K^{(-s)}$. Also, Euler's transform [11, Eqn. (2.2.7)] and a contiguous relation yield

$$E^{(-s)} = \frac{4s(1-k^2)}{2s-1} K^s + \frac{2s+1}{2s-1} E^s.$$

An integral form of K^s is given by

$$K^s(k) = \frac{\cos \pi s}{2} \int_0^1 \frac{t^{s-1/2}}{(1-t)^{1/2+s}(1-k^2 t)^{1/2-s}} dt. \quad (5.5)$$

This and many more forms for K^s, E^s can be obtained from <http://dlmf.nist.gov/15.6>. There are four values for which these integrals are truly special:

$$s \in \Omega := \left\{ 0, \frac{1}{6}, \frac{1}{4}, \frac{1}{3} \right\},$$

that is, when $\cos^2(\pi s)$ is rational. We return to these special values in Chapters 10 and 12. These give Ramanujan's alternative elliptic integrals as displayed in [164] and first decoded in [46]. A comprehensive study is given in [34] (see also [113] and [10]). These four cases all produce modular functions [46, §5.5], and there is currently a renewal of interest regarding related series for $1/\pi$ (e. g. [31], [70], [174] and [47]).

5.1.1. Series for π . Truly novel series for $1/\pi$, based on elliptic integrals, were discovered by Ramanujan around 1910 [31]. A famous one, with $s = 1/4$ is:

$$\frac{1}{\pi} = \frac{2\sqrt{2}}{9801} \sum_{k=0}^{\infty} \frac{4k! (1103 + 26390k)}{k!^4 396^{4k}}. \quad (5.6)$$

Each term of (5.6) adds eight correct digits. Gosper used (5.6) for the computation of a then-record 17 million digits of π in 1985 – thereby completing the first proof of (5.6) (based on the idea that algebraic numbers with bounded degree and height cannot be too close to each other numerically) [46, Ch. 3]. Shortly thereafter, David and Gregory Chudnovsky found the following variant, which uses $s = 1/3$ and lies in the quadratic field $\mathbb{Q}(\sqrt{-163})$ rather than $\mathbb{Q}(\sqrt{-58})$:

$$\frac{1}{\pi} = 12 \sum_{k=0}^{\infty} \frac{(-1)^k (6k)! (13591409 + 545140134k)}{(3k)! k!^3 640320^{3k+3/2}}. \quad (5.7)$$

Each term of (5.7) adds 14 correct digits. The Chudnovsky brothers used this formula several times, culminating in a 1994 calculation of π to over four billion decimal digits. Remarkably, (5.7) was used again in late 2009 for the then-record computation of π to 2.7 trillion places. A striking recent series due to Yang, see [209], is

$$\frac{1}{\pi} = \frac{\sqrt{15}}{18} \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 \frac{4n+1}{36^n}. \quad (5.8)$$

Further work has been done on similar series, see for example Chapter 12.

5.1.2. Classical results. A coupling equation between E^s and K^s is given in [46, p. 178]:

$$E^s = (1 - k^2) K^s + \frac{k(1 - k^2)}{1 + 2s} \frac{d}{dk} K^s. \quad (5.9)$$

Integrating this by parts leads to

$$K_{2,s} = \frac{(1 + 2s) E_{0,s} - 2s K_{0,s}}{2 - 2s}. \quad (5.10)$$

In the same fashion, multiplying by k^n before integrating the coupling provides a recursion for $K_{n+2,s}$:

$$K_{n+2,s} = \frac{(n - 2s) K_{n,s} + (1 + 2s) E_{n,s}}{n + 2(1 - s)}. \quad (5.11)$$

We also consider the *complementary* integrals:

$$K'^s(k) := K^s(\sqrt{1 - k^2}) \quad \text{and} \quad E'^s(k) := E^s(\sqrt{1 - k^2}).$$

The four integrals then satisfy a version of *Legendre's identity*,

$$E^s K'^s + K^s E'^s - K^s K'^s = \frac{\pi}{2} \frac{\cos \pi s}{1 + 2s} \quad (5.12)$$

for all $0 \leq s \leq 1$. We will come back to this amazing identity later in Chapters 6 and 12.

In [46, pp. 198–99] the moments are determined for the original complete elliptic integrals K and E . These are linked by the equations

$$E = (1 - k^2) K + k(1 - k^2) \frac{dK}{dk}, \quad (5.13)$$

which is (5.9) with $s = 0$ and

$$E = K + k \frac{dE}{dk}, \quad (5.14)$$

from which we derive the following recursions:

Theorem 5.1 ($s = 0$). For $n = 0, 1, 2, \dots$

$$(a) \quad K_{n+2} = \frac{nK_n + E_n}{n + 2} \quad \text{and} \quad (b) \quad E_n = \frac{K_n + 1}{n + 2}. \quad (5.15)$$

The recursion holds for real n . Moreover,

$$K_0 = 2G, \quad K_1 = 1, \quad E_0 = G + \frac{1}{2}, \quad E_1 = \frac{2}{3}. \quad (5.16)$$

Here

$$G := \sum_{n \geq 0} \frac{(-1)^n}{(2n+1)^2} = L_{-4}(2) \quad (5.17)$$

is *Catalan's constant* whose irrationality is still not proven. Indeed [3] uses the moment K_0 as a definition of G .

The current record for computation of G is 31.026 billion decimal digits in 2009. Computations often use the following central binomial formula due to Ramanujan [46, last formula] or its recent generalisations [62]:

$$\frac{3}{8} \sum_{n=0}^{\infty} \frac{1}{\binom{2n}{n}(2n+1)^2} + \frac{\pi}{8} \log(2 + \sqrt{3}) = G. \quad (5.18)$$

Early in 2011, a string of base-4096 digits of Catalan's constant beginning at position 10 trillion was computed on an IBM *Blue Gene/P* machine [22].

5.2. Basic results

We commence in this section with various fundamental representations and evaluations. Then in Section 3 we provide a generalisation of Catalan's constant arising as the expectation of K^s . In Section 4 we consider related contour integrals. Finally, in section 5 we look at negative and fractional moments.

5.2.1. Hypergeometric closed forms. A concise closed form for the moments is

Theorem 5.2 (Hypergeometric forms). *For $0 \leq s < \frac{1}{2}$ we have*

$$K_{n,s} = \frac{\pi}{2(n+1)} {}_3F_2 \left(\begin{matrix} \frac{1}{2} - s, \frac{1}{2} + s, \frac{n+1}{2} \\ 1, \frac{n+3}{2} \end{matrix} \middle| 1 \right), \quad (5.19)$$

$$E_{n,s} = \frac{\pi}{2(n+1)} {}_3F_2 \left(\begin{matrix} -\frac{1}{2} - s, \frac{1}{2} + s, \frac{n+1}{2} \\ 1, \frac{n+3}{2} \end{matrix} \middle| 1 \right). \quad (5.20)$$

These also hold in the limit for $s = \frac{1}{2}$.

PROOF. We use the following standard technique which makes use of the beta integral,

$$\beta(a, b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} = \int_0^1 t^{a-1}(1-t)^{b-1} dt. \quad (5.21)$$

After interchanging the order of summation and integration:

$$\begin{aligned} \int_0^1 x^{u-1}(1-x)^{v-1} {}_2F_1\left(a, 1-a \middle| b \middle| x\right) dx &= \sum_{n=0}^{\infty} \frac{(a)_n(1-a)_n}{(b)_n n!} \int_0^1 x^{n+u-1}(1-x)^{v-1} dx \\ &= \sum_{n=0}^{\infty} \frac{(a)_n(1-a)_n(u)_n}{(b)_n(u+v)_n n!} \frac{\Gamma(u)\Gamma(v)}{\Gamma(u+v)} \\ &= \frac{\Gamma(u)\Gamma(v)}{\Gamma(u+v)} {}_3F_2\left(a, 1-a, u \middle| b, u+v \middle| 1\right). \end{aligned} \quad (5.22)$$

Similarly,

$$\frac{\Gamma(u)\Gamma(v)}{\Gamma(u+v)} {}_3F_2\left(a, -a, u \middle| b, u+v \middle| 1\right) = \int_0^1 x^{u-1}(1-x)^{v-1} {}_2F_1\left(a, -a \middle| b \middle| x\right) dx.$$

By applying these to (5.1) and (5.2) we immediately get (5.19) and (5.20). \square

As long as $0 < s < 1/2$, the first series (5.19) is *Saalschützian* [179]. That is, the denominator parameters sum to one more than those in the numerator, but it is not well-poised, and can be reduced to Gamma functions only for $n = \pm 1$ since then it reduces to a ${}_2F_1$. The second (5.20) is not even Saalschützian, although it is nearly well-poised (see [179]) and also can be reduced to Gamma functions for $n = \pm 1$. Thus, for $|s| < 1/2$ we find

$$K_{1,s} = \frac{\cos \pi s}{1-4s^2}, \quad E_{1,s} = \frac{2}{2s+3} \frac{\cos \pi s}{1-4s^2}. \quad (5.23)$$

A cleaner form for $K_{n,0}$ is recorded in equation (7.21).

In what follows, we will be using the *digamma function*, given in terms of the Gamma function and the Euler-Mascheroni constant by:

$$\Psi(x) := \frac{\Gamma'(x)}{\Gamma(x)} = -\gamma + \sum_{n=1}^{\infty} \frac{x-1}{n(n+x-1)}. \quad (5.24)$$

(So $\Psi(1) = -\gamma$.) We prove:

Theorem 5.3 (Odd moments of K^s). *For odd integers $2m+1$ and $m = 0, 1, 2, \dots$,*

$$K_{2m+1,s} = \frac{\cos \pi s m!^2}{4 \Gamma\left(\frac{3}{2}-s+m\right) \Gamma\left(\frac{3}{2}+s+m\right)} \sum_{k=0}^m \frac{\Gamma\left(\frac{1}{2}-s+k\right) \Gamma\left(\frac{1}{2}+s+k\right)}{k!^2}. \quad (5.25)$$

PROOF. The *Legendre polynomial* (which we will more thoroughly investigate in Chapters 10, 11 and 12),

$$y = P_\nu(x) := {}_2F_1\left(-\nu, \nu+1 \middle| 1 \middle| \frac{1-x}{2}\right),$$

is a solution of the differential equation

$$(1-x^2)\frac{d^2y}{dx^2} - 2x\frac{dy}{dx} + \nu(\nu+1)y = 0.$$

In consequence we may deduce that

$${}_2F_1\left(\begin{matrix} a, 1-a \\ 1 \end{matrix} \middle| z\right) = \frac{\sin \pi a}{\pi} \sum_{k=0}^{\infty} \frac{(a)_k(1-a)_k}{k!^2} (1-z)^k \times \quad (5.26)$$

$$\{2\Psi(1+k) - \Psi(a+k) - \Psi(1-a+k) - \log(1-z)\},$$

using [138, p. 44, first formula ($b = 1 - a$)].

Now, by integrating the series (5.26) term-by-term and applying (5.22), we have

$${}_3F_2\left(\begin{matrix} a, 1-a, n \\ 1, n+1 \end{matrix} \middle| 1\right) = n \int_0^1 z^{n-1} {}_2F_1\left(\begin{matrix} a, 1-a \\ 1 \end{matrix} \middle| z\right) dz$$

$$= \frac{n! \sin \pi a}{\pi} \sum_{k=0}^{\infty} \frac{(a)_k(1-a)_k}{k!(k+n)!} \{\Psi(1+k) + \Psi(n+1+k) - \Psi(a+k) - \Psi(1-a+k)\}.$$

(This offers an apparently new approach for summing this class of hypergeometric series.) Then, by creative telescoping on the right hand side, one finds for any positive integer n ,

$${}_3F_2\left(\begin{matrix} a, 1-a, n \\ 1, n+1 \end{matrix} \middle| 1\right) = \frac{\Gamma(n)\Gamma(1+n)}{\Gamma(a+n)\Gamma(1-a+n)} \sum_{k=0}^{n-1} \frac{(a)_k(1-a)_k}{k!^2}. \quad (5.27)$$

Now, with $n = m + 1$ in (5.27), we conclude the proof of Theorem 5.3. \square

For $m = 0$, Theorem 5.3 reduces to the evaluation given in (5.23). A prettier partial fraction decomposition is

$$K_{2m+1,s} = \frac{\cos \pi s}{2} \sum_{k=0}^m \frac{m!^2}{(m-k)!(m+k+1)!} \left(\frac{1}{2k+1-2s} + \frac{1}{2k+1+2s} \right), \quad (5.28)$$

which can easily be confirmed inductively, using (5.65) below.

For $s = 0$ the result of Theorem 5.3 originates with Ramanujan. Adamchik [3] reprises its substantial history and extensions which include a formula due independently to Bailey and Hodgkinson in 1931 and which subsumes (5.27). A special case of Bailey's formula is

$${}_3F_2\left(\begin{matrix} a, b, c+n-1 \\ a+b+n, c \end{matrix} \middle| 1\right) = \frac{\Gamma(n)\Gamma(a+b+n)}{\Gamma(a+n)\Gamma(b+n)} \sum_{k=0}^{n-1} \frac{(a)_k(b)_k}{(c)_k(1)_k}. \quad (5.29)$$

This identity, once found, can be easily checked by Zeilberger's algorithm.

Example 5.2.1 (Odd moments of E^s). The corresponding form for $E_{2m+1,s}$ is

$$E_{2m-1,s} = \frac{\cos \pi s}{2(s+m)+1} \left\{ \frac{1}{2s+1} + \sum_{k=0}^{m-1} \frac{(m-1)!^2}{(m-1-k)!(m+k)!} \frac{(2s+1)(2k+1)}{(2k+1)^2 - 4s^2} \right\}, \quad (5.30)$$

on combining (5.25) with (5.66) below. \diamond

Example 5.2.2 (Digamma consequences). For $0 < a < 1/2$, we use

$$\gamma(\nu) := \frac{1}{2} \left[\Psi \left(\frac{\nu+1}{2} \right) - \Psi \left(\frac{\nu}{2} \right) \right],$$

for which

$$\begin{aligned} \gamma \left(\frac{1}{2} \right) &= \frac{\pi}{2}, & \gamma \left(\frac{1}{4} \right) &= \frac{\pi}{\sqrt{2}} - \sqrt{2} \log(\sqrt{2} - 1), \\ \gamma \left(\frac{1}{3} \right) &= \frac{\pi}{\sqrt{3}} + \log 2, & \gamma \left(\frac{1}{6} \right) &= \pi + \sqrt{3} \log(2 + \sqrt{3}). \end{aligned}$$

More generally,

$$\begin{aligned} & \sum_{k=0}^{\infty} \frac{(a)_k (1-a)_k}{\left(\frac{3}{2}\right)_k k!} \left[\Psi(k+1) + \Psi \left(k + \frac{3}{2} \right) - \Psi(k+a) - \Psi(k+1-a) \right] \\ &= \frac{2\gamma(a) - \pi \csc(\pi a)}{1-2a}. \end{aligned}$$

This in turn gives

$${}_3F_2 \left(\begin{matrix} a, 1-a, \frac{1}{2} \\ 1, \frac{3}{2} \end{matrix} \middle| 1 \right) = \frac{2 \sin(\pi a)}{\pi(1-2a)} \gamma(a) - \frac{1}{1-2a}. \quad (5.31)$$

Taking the limit as $a \rightarrow 1/2$ in (5.31) gives two useful specialisations:

$${}_3F_2 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, \frac{3}{2} \end{matrix} \middle| 1 \right) = \frac{4G}{\pi}, \quad \Psi' \left(\frac{1}{4} \right) = \pi^2 + 8G. \quad (5.32)$$

\diamond

Example 5.2.3 (Half-integer values of s). For $s = m + 1/2$, and $m, n = 0, 1, 2, \dots$ we can obtain a terminating representation using Saalschütz's theorem (14.10),

$$\begin{aligned} K_{n,m+1/2} &= \frac{\pi}{2(n+1)} {}_3F_2 \left(\begin{matrix} -m, m+1, \frac{n+1}{2} \\ 1, \frac{n+3}{2} \end{matrix} \middle| 1 \right) \\ &= \frac{(-1)^m \pi}{4} \frac{\Gamma^2 \left(\frac{n+1}{2} \right)}{\Gamma \left(\frac{n+1}{2} - m \right) \Gamma \left(\frac{n+3}{2} + m \right)}, \end{aligned} \quad (5.33)$$

and likewise

$$E_{n,m+1/2} = \frac{(-1)^m (m+1) \pi}{4} \frac{\Gamma^2 \left(\frac{n+1}{2} \right)}{\Gamma \left(\frac{n+1}{2} - m \right) \Gamma \left(\frac{n+5}{2} + m \right)}, \quad (5.34)$$

by equation (14.12) in Chapter 14. \diamond

5.2.2. The complementary integrals. By contrast, the complementary integral moments are less recondite.

Theorem 5.4 (Complementary moments). *For $n = 0, 1, 2, \dots$ and $0 \leq s < \frac{1}{2}$,*

$$K'_{n,s} = \frac{\pi}{4} \frac{\Gamma^2\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{n+2-2s}{2}\right)\Gamma\left(\frac{n+2+2s}{2}\right)}, \quad (5.35)$$

$$E'_{n,s} = \frac{\pi}{2(n+1)} \frac{\Gamma^2\left(\frac{n+3}{2}\right)}{\Gamma\left(\frac{n+2-2s}{2}\right)\Gamma\left(\frac{n+4+2s}{2}\right)}. \quad (5.36)$$

These also hold in the limit for $s = \frac{1}{2}$.

In particular, we recursively obtain for all real n :

$$(a) K'_{n+2,s} = \frac{(n+1)^2}{(n+2)^2 - 4s^2} K'_{n,s}, \quad (b) E'_{n,s} = \frac{n+1}{n+2+2s} K'_{n,s}, \quad (5.37)$$

$$\text{with (c) } K'_{0,s} = \frac{\pi}{4} \frac{\sin(\pi s)}{s}, \quad (d) \quad K'_{1,s} = \frac{\cos \pi s}{1 - 4s^2}.$$

PROOF. To establish (5.35) we recall that

$$K^{s'} = \frac{\pi}{2} {}_2F_1\left(\frac{1}{2} - s, \frac{1}{2} + s \middle| 1 - k^2\right), \quad (5.38)$$

and so

$$\begin{aligned} K'_{n,s} &= \frac{\pi}{2} \int_0^1 x^n {}_2F_1\left(\frac{1}{2} - s, \frac{1}{2} + s \middle| 1 - x^2\right) dx \\ &= \frac{\pi}{4} \int_0^1 (1-x)^{\frac{n+1}{2}-1} {}_2F_1\left(\frac{1}{2} - s, \frac{1}{2} + s \middle| x\right) dx \\ &= \frac{\pi}{2(n+1)} {}_3F_2\left(\frac{1}{2} - s, \frac{1}{2} + s, 1 \middle| 1\right) = \frac{\pi}{2(n+1)} {}_2F_1\left(\frac{1}{2} - s, \frac{1}{2} + s \middle| \frac{n+3}{2}\right), \end{aligned}$$

which is summable, by Gauss' formula (5.3), to the desired result.

The proof of (5.36) is similar, and the recursions follow. \square

Example 5.2.4 (Complementary closed forms). With $s = 0$ and $n = 0, 1$ we recover

$$K'_0 = \frac{\pi^2}{4}, \quad E'_0 = \frac{\pi^2}{8}, \quad K'_1 = 1, \quad E'_1 = \frac{2}{3},$$

as discussed in [46, p. 198]. Correspondingly

$$\begin{aligned} K'_{0,1/6} &= \frac{3\pi}{4}, & K'_{1,1/6} &= \frac{9\sqrt{3}}{16}, & E'_{0,1/6} &= \frac{9\pi}{28}, & K'_{1,1/6} &= \frac{27\sqrt{3}}{80}, \\ K'_{0,1/3} &= \frac{3\sqrt{3}\pi}{8}, & K'_{1,1/3} &= \frac{9}{10}, & E'_{0,1/3} &= \frac{9\sqrt{3}\pi}{64}, & E'_{1,1/3} &= \frac{27}{55}. \end{aligned}$$

We note that π , not π^2 appears in these evaluations, since in (5.37, c), $\sin(\pi s)/s \rightarrow \pi$ as $s \rightarrow 0$. \diamond

We note that a comparison of Theorems 5.3 and 5.4 shows that (trivially)

$$K'_{1,s} = K_{1,s} \quad \text{and} \quad E'_{1,s} = E_{1,s}.$$

Remark 5.2.1. The formula

$$\int_0^1 K(k) \frac{dk}{1+k} = \int_0^1 K\left(\frac{1-h}{1+h}\right) \frac{dh}{1+h} = \frac{1}{2} \int_0^1 K'(k) dk \quad (5.39)$$

is recorded in [46, p. 199]. It is proven by using the quadratic transform [46, Thm 1.2 (b)] for the second equality and a substitution for the first. This implies

$$2 \sum_{n=0}^{\infty} (-1)^n K_n = \frac{\pi^2}{4} = K'_0, \quad (5.40)$$

on appealing to Theorem 5.4.

The corresponding identity for $s = 1/6$ is best written as

$$\int_0^1 {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \middle| 1-t^3\right) dt = 3 \int_0^1 {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \middle| t^3\right) \frac{dt}{1+2t}, \quad (5.41)$$

which follows analogously from the cubic transformation [45, (2.1)] and a change of variables. This is a beautiful counterpart to (5.39), especially when the latter is written in hypergeometric form:

$$\int_0^1 {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| 1-k^2\right) dk = 2 \int_0^1 {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| k^2\right) \frac{dk}{1+k}. \quad (5.42)$$

Additionally, [46, p. 188] outlines how to derive

$$\int_0^1 \frac{K(k) dk}{\sqrt{1-k^2}} = K\left(\frac{1}{\sqrt{2}}\right)^2.$$

Using the same technique, we generalise this to

$$\int_0^1 \frac{K^s(k) dk}{\sqrt{1-k^2}} = K^s\left(\frac{1}{\sqrt{2}}\right)^2 = \frac{\cos^2(\pi s)}{16\pi} \Gamma^2\left(\frac{1+2s}{4}\right) \Gamma^2\left(\frac{1-2s}{4}\right). \quad (5.43)$$

Here we have used Gauss' formula (5.3) for the evaluation of $K^s(1/\sqrt{2})$. By the generalised Legendre's identity (5.12), which simplifies as the complementary integrals coincide with the original ones at $1/\sqrt{2}$, we obtain

$$E^s\left(\frac{1}{\sqrt{2}}\right) = \frac{K^s\left(\frac{1}{\sqrt{2}}\right)}{2} + \frac{\pi \cos \pi s}{4(2s+1)K^s\left(\frac{1}{\sqrt{2}}\right)}.$$

\diamond

5.3. Closed form initial values

Empirically, we discovered the algebraic relation

$$2(1+s)E_{0,s} - (1+2s)K_{0,s} = \frac{\cos \pi s}{1+2s}. \quad (5.44)$$

On using (5.10) to eliminate $E_{0,s}$ in (5.44), it becomes

$$K_{2,s} = \frac{K_{0,s} + \cos(\pi s)}{4 - 4s^2} \quad (5.45)$$

which in turn is a special case of (5.65) below with $r = \frac{1}{2}$ (as is justified by Carlson's Theorem 1.3), thus proving our empirical observation.

Hence, to resolve all integral values for a given s , we are left with looking for satisfactory representations only for $K_{0,s}$. We will write

$$G_s := \frac{1}{2}K_{0,s} = \frac{\pi}{4} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2} - s, \frac{1}{2} + s \\ 1, \frac{3}{2} \end{matrix} \middle| 1\right) \quad (5.46)$$

and call this the *generalised Catalan constant*.

5.3.1. Evaluation of G_s . From (5.19) we obtain

$$\begin{aligned} K_{0,s} &= \frac{\pi}{2} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2} - s, \frac{1}{2} + s \\ 1, \frac{3}{2} \end{matrix} \middle| 1\right) = \frac{\cos \pi s}{2} \sum_{n=0}^{\infty} \frac{\Gamma(\frac{1}{2} + n + s) \Gamma(\frac{1}{2} + n - s)}{(2n+1)n!^2} \\ &= \frac{\cos \pi s}{2} \sum_{n=0}^{\infty} \beta\left(n + \frac{1}{2} - s, n + \frac{1}{2} + s\right) \frac{\binom{2n}{n}}{2n+1} \\ &= \frac{\cos \pi s}{4} \int_0^1 \frac{\arcsin(2\sqrt{t-t^2})}{t^{1+s}(1-t)^{1-s}} dt \\ &= \frac{\cos \pi s}{2} \int_0^{\pi/2} \left\{ \tan^{2s}\left(\frac{\theta}{2}\right) + \cot^{2s}\left(\frac{\theta}{2}\right) \right\} \frac{\theta}{\sin \theta} d\theta. \end{aligned} \quad (5.47)$$

Here we again write the Gamma terms as a beta integral, and exchange the order of integration and summation, followed by various trigonometric substitutions. For example, we have

$$K_{0,0} = \int_0^{\pi/2} \frac{\theta}{\sin \theta} d\theta = 2G.$$

The final equality has various derivations [46, 3]; these include contour integration as explored in Section 5.4.

If we now make the trigonometric substitution $t = \tan(\theta/2)$ in (5.47), and integrate the two resulting terms separately, we arrive at the following evaluation.

Theorem 5.5 (Generalised Catalan constants). *For $0 \leq s \leq \frac{1}{2}$, we have*

$$\begin{aligned} K_{0,s} &= \cos \pi s \int_0^1 (t^{2s-1} + t^{-2s-1}) \arctan t \, dt \\ &= \frac{\cos \pi s}{8s} \left\{ \Psi\left(\frac{3-2s}{4}\right) + \Psi\left(\frac{1+2s}{4}\right) - \Psi\left(\frac{1-2s}{4}\right) - \Psi\left(\frac{3+2s}{4}\right) \right\} \\ &= \frac{\cos \pi s}{4s} \left\{ \Psi\left(\frac{s}{2} + \frac{1}{4}\right) - \Psi\left(\frac{s}{2} + \frac{3}{4}\right) \right\} + \frac{\pi}{4s} = 2G_s. \end{aligned} \quad (5.48)$$

Note that for $s = 0$, applying L'Hôpital's rule to (5.48) yields

$$K_{0,0} = \frac{1}{8} \Psi' \left(\frac{1}{4} \right) - \frac{1}{8} \Psi' \left(\frac{3}{4} \right)$$

which is precisely $2G$.

The digamma expression in (5.48) simplifies entirely when $s \in \Omega$.

Corollary 5.1 (generalised Catalan values for $s \in \Omega$).

$$G_0 = G, \quad G_{1/6} = \frac{3\sqrt{3}}{4} \log 2, \quad G_{1/4} = \log(1 + \sqrt{2}), \quad G_{1/3} = \frac{3\sqrt{3}}{8} \log(2 + \sqrt{3}). \quad (5.49)$$

Mathematica, which currently knows more about the Ψ function than *Maple*, can evaluate the integral in Theorem 5.5 symbolically for some s . For example, for $s = 1/12$, after simplification we get

$$G_{1/12} = 3(\sqrt{3} + 1) \left\{ \log(\sqrt{2} - 1) + \frac{\sqrt{3}}{2} \log(\sqrt{3} + \sqrt{2}) \right\}.$$

More generally, the evaluation requires only knowledge of $\sin(\pi s/2)$, and hence we can determine which s gives a reduction to radicals. As a last example,

$$G_{1/5} = \frac{5}{8} \sqrt{5 + 2\sqrt{5}} \left\{ \frac{\sqrt{5} - 1}{2} \operatorname{arcsinh} \left(\sqrt{5 + 2\sqrt{5}} \right) - \operatorname{arcsinh} \left(\sqrt{5 - 2\sqrt{5}} \right) \right\}.$$

5.3.2. Other generalisations of G . Other famous representations of G include

$$G = - \int_0^{\pi/2} \log \left(2 \sin \frac{t}{2} \right) dt \quad (5.50)$$

$$= \int_0^{\pi/2} \log \left(2 \cos \frac{t}{2} \right) dt, \quad (5.51)$$

$$\text{and } G = - \int_0^{\pi/2} \log(\tan t) dt, \quad (5.52)$$

which easily follow from (5.50) and (5.51). To prove (5.50), which is an example of a log-sin integral more carefully studied in Chapter 9, we integrate by parts and obtain

$$\begin{aligned}
-\int_0^{\pi/2} \log\left(2 \sin \frac{t}{2}\right) dt &= 2 \int_0^{\pi/4} t \cot t dt - \frac{\pi}{4} \log 2 \\
&= 2 \int_0^{\pi/4} {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| \frac{3}{2} \middle| \sin^2 t\right) \cos t dt - \frac{\pi}{4} \log 2 \\
&= 2 \int_0^{1/\sqrt{2}} \frac{\arcsin x}{x} dx - \frac{\pi}{4} \log 2 \\
&= \left(G + \frac{\pi}{4} \log 2\right) - \frac{\pi}{4} \log 2 = G.
\end{aligned}$$

The second and third equalities hold since $x {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; \frac{3}{2}; x^2\right) = \arcsin x$. The final equality follows on integrating $\arcsin(x)/x$ term by term. Inter alia, we have shown that

$$2G = \int_0^{\pi/2} \frac{t}{\sin t} dt = \int_0^{\pi/2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| \frac{3}{2} \middle| \sin^2 t\right) dt. \quad (5.53)$$

We may generalise (5.50) or equivalently (5.53) to:

Proposition 5.1.

$$G_s = \frac{\cos \pi s}{2} \int_0^{\pi/2} \tan^{2s} t {}_2F_1\left(\frac{1}{2}, \frac{1}{2} - s \middle| \frac{3}{2} \middle| \sin^2 t\right) dt. \quad (5.54)$$

PROOF. We write

$$\begin{aligned}
G_s &= \frac{1}{2} \int_0^1 K^s(k) dk = \frac{\pi}{4} \int_0^1 {}_2F_1\left(\frac{1}{2} - s, \frac{1}{2} + s \middle| 1 \middle| k^2\right) dk \\
&= \frac{\cos \pi s}{4} \int_0^1 t^{s-1/2} (1-t)^{-s-1/2} dt \int_0^1 (1-k^2 t)^{s-1/2} dk \\
&= \frac{\cos \pi s}{4} \int_0^1 t^{s-1/2} (1-t)^{-s-1/2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2} - s \middle| \frac{3}{2} \middle| t\right) dt \\
&= \frac{\cos \pi s}{2} \int_0^{\pi/2} \tan^{2s} u {}_2F_1\left(\frac{1}{2}, \frac{1}{2} - s \middle| \frac{3}{2} \middle| \sin^2 u\right) du.
\end{aligned}$$

□

Note that from Theorem 5.2 and (5.31), we recover Theorem 5.5 in the equivalent form

$$G_s = \frac{\pi}{4} {}_3F_2\left(\frac{1}{2} - s, \frac{1}{2} + s, \frac{1}{2} \middle| 1\right) = \frac{\cos \pi s}{4s} \gamma\left(\frac{1}{2} + s\right) - \frac{\pi}{8s}. \quad (5.55)$$

5.4. Contour integrals for G_s

By contour integration of $t/\sin t$ on the infinite rectangle above $[0, \pi/2]$, we obtain

$$G_0 = \frac{1}{2} \int_0^\infty \frac{t}{\cosh t} dt = \int_0^\infty \frac{te^{-t}}{1+e^{-2t}} dt = \sum_{n \geq 0} \frac{(-1)^n}{(2n+1)^2} = G. \quad (5.56)$$

Here we have used the geometric series and integrated term by term.

Done carefully, contour integration over the same rectangle, converting to exponentials, and then integrating term by term, provides a general integral evaluation:

Lemma 5.1 (Contour integral for G_s). *For $0 \leq s < 1/2$ we have*

$$\begin{aligned} 2G_s = K_{0,s} &= 2^{2s} \sin(2\pi s) \int_0^\infty \frac{\cosh^{4s} t - \sinh^{4s} t}{\sinh^{2s+1} 2t} t dt \\ &\quad + \cos(\pi s) \int_0^\infty \frac{\cos(2s \arctan(\sinh t))}{\cosh t} t dt. \end{aligned} \quad (5.57)$$

Now write (5.57) as

$$K_{0,s} = \sin(2\pi s) S(s) + \cos(\pi s) C(s). \quad (5.58)$$

To evaluate $S(s)$ we make a substitution $u = \tanh(t)$. We obtain

$$\begin{aligned} S(s) &= \frac{1}{2} \int_0^1 (u^{-2s-1} - u^{2s-1}) \operatorname{arctanh}(u) du \\ &= \frac{-1}{8s} \left(2\gamma + 4 \log(2) + \Psi\left(\frac{1}{2} - s\right) + \Psi\left(\frac{1}{2} + s\right) \right). \end{aligned} \quad (5.59)$$

To evaluate $C(s)$ we note that

$$\cos(2s \arctan(\sinh t)) = \cos(2s \arcsin(\tanh t)) = {}_2F_1\left(\begin{matrix} s, -s \\ \frac{1}{2} \end{matrix} \middle| \tanh^2 t\right) \quad (5.60)$$

and so we obtain a converging series

$$C(s) = \int_0^\infty \frac{\cos(2s \arctan(\sinh t))}{\cosh t} t dt = \sum_{n=0}^\infty \frac{(s)_n (-s)_n}{\left(\frac{1}{2}\right)_n} \frac{\tau_n}{n!}$$

where

$$\tau_n := \int_0^\infty \frac{x^{2n}}{(1+x^2)^{n+1}} \operatorname{arcsinh}(x) dx.$$

Moreover,

$$\tau_{m+2} = \frac{(13 + 8m^2 + 20m) \tau_{m+1} - 2(m+1)(2m+1) \tau_m}{2(m+2)(2m+3)} \quad (5.61)$$

where $\tau_0 = K_0 = 2G$ and $\tau_1 = E_0 = G + \frac{1}{2}$. In particular $C(0) = 2G$.

A closed form for τ_n is easily obtained by creative telescoping. It is

$$\tau_n = \beta\left(n + \frac{1}{2}, \frac{1}{2}\right) \left\{ \frac{2G}{\pi} + \frac{1}{4} \sum_{k=1}^n \frac{\Gamma^2(k)}{\Gamma^2\left(k + \frac{1}{2}\right)} \right\}. \quad (5.62)$$

Collecting up evaluations, we deduce that

$$K_{0,s} = \sin(2\pi s) \left\{ \frac{-1}{8s} \left(2\gamma + 4 \log(2) + \Psi\left(\frac{1}{2} - s\right) + \Psi\left(\frac{1}{2} + s\right) \right) \right\} + \frac{\sin(2\pi s)}{\pi s} \left\{ G - \pi \sum_{k=0}^{\infty} \frac{\Gamma(k+s+1)\Gamma(k-s+1) - k!^2}{8\Gamma\left(k + \frac{3}{2}\right)^2} \right\}.$$

This ultimately yields:

Theorem 5.6 (Contour series for G_s).

$$G_s = \frac{\sin 2\pi s}{16s} \left[\sum_{k=1}^{\infty} \frac{\Gamma^2(k) - \Gamma(k+s)\Gamma(k-s)}{\Gamma^2\left(k + \frac{1}{2}\right)} + 2\Psi\left(\frac{1}{2}\right) - 2\Psi\left(s + \frac{1}{2}\right) + \pi \tan(\pi s) + \frac{8G}{\pi} \right]. \quad (5.63)$$

5.5. Closed forms at negative integers

We observe that (5.19) and (5.20) give analytic continuations which allow us to study negative moments. In [3] Adamchik studies such moments of K .

5.5.1. Negative moments. Adamchik's starting point is the study of $K_n = K_{n,0}$, for which Ramanujan appears to have known that

$$(2r+1)^2 K_{2r+1} - (2r)^2 K_{2r-1} = 1, \quad (5.64)$$

for $\operatorname{Re} r > -1/2$. For integer r this is a direct consequence of (5.25).

Experimentally, we found the following extension for general s by using integer relation methods with $s := 1/n$ to determine the coefficients:

$$((2r+1)^2 - 4s^2) K_{2r+1,s} - (2r)^2 K_{2r-1,s} = \cos \pi s. \quad (5.65)$$

For integer r this is established as follows – the general case then follows by Carlson's Theorem 1.3. Using (5.25) and the functional relation for the Γ function, we have:

$$\begin{aligned} & ((2r+1)^2 - 4s^2) K_{2r+1,s} - 4r^2 K_{2r-1,s} \\ &= \frac{\pi r!^2}{\Gamma\left(\frac{1}{2} + r - s\right)\Gamma\left(\frac{1}{2} + r + s\right)} \left\{ \sum_{k=0}^r \frac{\left(\frac{1}{2} - s\right)_k \left(\frac{1}{2} + s\right)_k}{k!^2} - \sum_{k=0}^{r-1} \frac{\left(\frac{1}{2} - s\right)_k \left(\frac{1}{2} + s\right)_k}{k!^2} \right\} \\ &= \frac{\pi r!^2}{\Gamma\left(\frac{1}{2} + r - s\right)\Gamma\left(\frac{1}{2} + r + s\right)} \frac{\left(\frac{1}{2} - s\right)_r \left(\frac{1}{2} + s\right)_r}{r!^2} = \cos(\pi s). \end{aligned}$$

Equation (5.11), when combined with (5.65), implies

$$E_{n,s} = \frac{(2s+1)^2 K_{n,s} + \cos \pi s}{(2s+1)(2s+n+2)}, \quad (5.66)$$

which extends (5.15) and completes the proof in Example 5.2.1.

Remark 5.5.1 (Terminating sums). While studying [3] we distilled the following.

(1) For $0 < a \leq 1$

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, a \\ 1, 1+a \end{matrix} \middle| 1\right) = \frac{4a}{\pi} {}_3F_2\left(\begin{matrix} 1, 1, 1-a \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right). \quad (5.67)$$

In particular, when $a = 1/2$ or $1/4$,

$$\begin{aligned} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, \frac{3}{2} \end{matrix} \middle| 1\right) &= \frac{2}{\pi} {}_3F_2\left(\begin{matrix} 1, 1, \frac{1}{2} \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) = \frac{4}{\pi} G, \\ {}_3F_2\left(\begin{matrix} \frac{3}{4}, 1, 1 \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) &= \frac{\Gamma^4(\frac{1}{4})}{16\pi}, \end{aligned}$$

the last evaluation takes advantage of Dixon's theorem (14.14).

(2) Moreover, for $n = 1, 2, 3, \dots$

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, n \\ 1, 1+n \end{matrix} \middle| 1\right)$$

always terminates (this is a specialisation of (5.29)). For example,

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, 1 \\ 1, 2 \end{matrix} \middle| 1\right) = \frac{4}{\pi}.$$

(3) Also for $n = 1, 2, \dots$

$$\begin{aligned} (2n+1)^2 {}_3F_2\left(\begin{matrix} 1, 1, -n \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) - 4n^2 {}_3F_2\left(\begin{matrix} 1, 1, 1-n \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) &= 1, \\ {}_3F_2\left(\begin{matrix} 1, 1, 1-n \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) &= \frac{4^{2n-1}}{n^2 \binom{2n}{n}^2} \sum_{k=0}^{n-1} \frac{\binom{2k}{k}^2}{4^{2k}}, \\ {}_3F_2\left(\begin{matrix} 1, 1, \frac{1}{2}-n \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) &= \frac{\binom{2n}{n}^2}{4^{2n}} \left\{ 2G + \sum_{k=0}^{n-1} \frac{4^{2k}}{\binom{2k}{k}^2 (2k+1)^2} \right\}. \end{aligned}$$

(4) For $0 < a \leq 1$ and $n = 1, 2, \dots$

$${}_3F_2\left(\begin{matrix} 1, 1, 1-n-a \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) = \frac{(a)_n^2}{(a+\frac{1}{2})_n^2} \left\{ {}_3F_2\left(\begin{matrix} 1, 1, 1-a \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) + \frac{1}{4a^2} \sum_{k=0}^{n-1} \frac{(a+\frac{1}{2})_k^2}{(a+1)_k^2} \right\}.$$

(5) Finally,

$$\sum_{k=0}^n \frac{(-1)^k k!}{\Gamma^2(k+\frac{3}{2})(n-k)!} = \frac{n!}{\pi \Gamma^2(n+\frac{3}{2})} \sum_{k=0}^n \frac{\Gamma^2(k+\frac{1}{2})}{k!^2}.$$

◇

5.5.2. Analyticity of $K_{r,s}$ for $0 \leq s < 1/2$. The analytic structure of $r \mapsto K_{r,s}$ is similar qualitatively for all s . There are simple poles at odd negative integers with computable residues.

Theorem 5.7 (Poles of $K_{r,s}$). *Let $R_{n,s}$ denote the residue of $K_{r,s}$ at $r = -2n + 1$.*

Then

$$(a) R_{n+1,s} = \frac{(n - \frac{1}{2})^2 - s^2}{n^2} R_{n,s}, \quad (b) R_{1,s} = \frac{\pi}{2}. \quad (5.68)$$

Explicitly

$$(c) R_{n,s} = \frac{\cos \pi s \Gamma(n - \frac{1}{2} + s) \Gamma(n - \frac{1}{2} - s)}{2 \Gamma^2(n)}. \quad (5.69)$$

PROOF. Recursion (5.68, a) follows from multiplying (5.65) by $2(r+n) = (2r+1) - (1-2n)$ and computing the limits as $r \rightarrow -n$.

Directly from Theorem 5.2, we have

$$R_{1,s} = \frac{\pi}{2} \lim_{r \rightarrow -1} \frac{r+1}{r+1} {}_3F_2 \left(\begin{matrix} \frac{1}{2} - s, \frac{1}{2} + s, \frac{r+1}{2} \\ 1, \frac{r+3}{2} \end{matrix} \middle| 1 \right) = \frac{\pi}{2},$$

which is (b); part (c) follows easily as a telescoping product. \square

5.5.3. Other rational values of s . For $s = 0$ only, $K_{-1/2,s}$ reduces to a case of Dixon's theorem and yields

$$K_{-1/2,0} = \frac{\Gamma^4(\frac{1}{4})}{16\pi}, \quad (5.70)$$

a result known to Ramanujan. A closed form is also possible for $K'_{-1/3,1/6}$, or equivalently

$$H = \frac{\pi}{2} \int_0^1 {}_2F_1 \left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| 1 - t^3 \right) dt. \quad (5.71)$$

We first write

$$H = \frac{\pi}{6} \int_0^1 x^{-\frac{2}{3}} {}_2F_1 \left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| 1 - x \right) dx = \frac{\pi}{6} \int_0^1 (1-x)^{-\frac{2}{3}} {}_2F_1 \left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| x \right) dx.$$

Now the integral (5.22) shows this is $\frac{\pi}{2} {}_2F_1(\frac{1}{3}, 1; \frac{4}{3}, 1)$. By Gauss' formula (5.3) we arrive at

$$H = \frac{\sqrt{3}}{12} \Gamma^3\left(\frac{1}{3}\right). \quad (5.72)$$

This also follows directly from the analytic continuation of the formula (5.35).

Moments of Products of Elliptic Integrals

ABSTRACT. We consider the moments of products of complete elliptic integrals of the first and second kinds. In particular, we derive new results using a variety of means, aided by computer experimentation and a theorem of Zudilin (which has been used in Chapter 2).

6.1. Motivation and general approach

We recall the definitions of the complete elliptic integral of the first kind $K(x)$, and the second kind $E(x)$:

Definition 6.1.

$$K(x) = \frac{\pi}{2} {}_2F_1\left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| x^2\right), \quad E(x) = \frac{\pi}{2} {}_2F_1\left(\begin{matrix} -\frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| x^2\right); \quad (6.1)$$

$$K(x) = \int_0^{\pi/2} \frac{dt}{\sqrt{1-x^2\sin^2 t}}, \quad E(x) = \int_0^{\pi/2} \sqrt{1-x^2\sin^2 t} dt. \quad (6.2)$$

As usual, $K'(x) = K(x')$, $E'(x) = E(x')$, where $x' = \sqrt{1-x^2}$.

The complete elliptic integrals, apart from their theoretical importance in arbitrary precision numerical computations [46] and the theory of theta functions (see also Chapters 10 – 12), are also of significant interest in applied fields such as electrodynamics, statistical mechanics, and random walks [56, 57]. They associate in many ways with various lattices [110]. K and E were first used to provide explicit solutions to the perimeter of an ellipse (among other curves) as well as the exact period of an ideal pendulum. They can be used to integrate algebraic expressions involving square roots of cubic or quartic polynomials (e.g. see Chapter 4). Their properties were investigated by Wallis, Landen, Fagnano, Euler, Lagrange, Legendre, Gauss, Jacobi, among others; many such properties are recorded on the general reference site <http://functions.wolfram.com>.

The author was first drawn to the study of integral of products of K and E in [56] (Chapter 2), in which it is shown that

$$2 \int_0^1 K(x)^2 dx = \int_0^1 K'(x)^2 dx, \quad (6.3)$$

by relating both sides to a moment of the distance from the origin in a four step uniform random walk on the plane. A much less recondite proof was only found later: set $x = (1 - t)/(1 + t)$ on the left hand side of (6.3), and apply the quadratic transform (6.4) below, and the result readily follows.

The four quadratic transforms [46], which we will use over and over, are:

$$K'(x) = \frac{2}{1+x} K\left(\frac{1-x}{1+x}\right) \quad (6.4)$$

$$K(x) = \frac{1}{1+x} K\left(\frac{2\sqrt{x}}{1+x}\right) \quad (6.5)$$

$$E'(x) = (1+x)E\left(\frac{1-x}{1+x}\right) - xK'(x) \quad (6.6)$$

$$E(x) = \frac{1+x}{2} E\left(\frac{2\sqrt{x}}{1+x}\right) + \frac{1-x^2}{2} K(x). \quad (6.7)$$

In the following sections we will consider definite integrals involving products of K, E, K', E' , especially the moments of the products, as a continuation of our study in Chapter 5. A goal of this chapter is to produce closed forms for these integrals whenever possible. When this is not achieved, closed forms for certain linear combinations of integrals are instead obtained. Thus, we are able to prove a large number of experimentally observed identities in [19].

The somewhat rich and unexpected results lend themselves for easy discovery, thanks to the methods of experimental mathematics: for instance, the *integer relations algorithm* PSLQ [91], the *Inverse Symbolic Calculator* (ISC, hosted at Newcastle, <http://isc.carma.newcastle.edu.au/>), the *Online Encyclopedia of Integer Sequences* (OEIS, [180]), the *Maple* package `gfun`, *Gosper's algorithm* (which finds closed forms for indefinite sums of hypergeometric terms, [161]), and Sister Celine's method [161]. Indeed, large scale computer experiments [19] reveal that there is a huge number of identities in the flavour of (6.3). Once discovered, many results can be routinely established by the following elementary techniques:

- (1) Connections with and transforms of hypergeometric and Meijer G-functions (see also Chapter 2), as in the case of random walk integrals (Section 6.3).

- (2) Interchange order of summation and integration, which is justified as all terms in the relevant series are positive (Section 6.4) (we may use either the series or the integrals for E or K).
- (3) Change the variable x to x' , usually followed by a quadratic transform (Section 6.5).
- (4) Use a Fourier series originally due to Tricomi (Section 6.6).
- (5) Apply Legendre's relation (Section 6.7).
- (6) Differentiate a product and integrate by parts (Section 6.8).

Section 6.2 and most of Section 6.7 are expository. The propositions in Section 6.4 are well-known, but the arithmetic nature of the moments, Theorem 6.3 and Lemma 6.3 in Section 6.6 seem to be original. Section 6.3 contains new general formulas for the moments of the product of two elliptic integrals, and Section 6.8 contains many new, though mostly easy, linear relations between the moments. Some useful identities of elliptic integrals are also gathered throughout the chapter.

6.2. One elliptic integral

The moments of a single K, E, K', E' are well known (e. g. see [46]). For completeness here we state a slightly more general result.

It follows by a straightforward application of the beta integral (5.21) that

$$\int_0^1 x'^m x^m K(x) dx = \frac{\pi \Gamma(\frac{1}{2}(m+1)) \Gamma(\frac{1}{2}(n+2))}{4 \Gamma(\frac{1}{2}(m+n+3))} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{m+1}{2} \\ 1, \frac{m+n+3}{2} \end{matrix} \middle| 1\right), \quad (6.8)$$

$$\int_0^1 x'^m x^m E(x) dx = \frac{\pi \Gamma(\frac{1}{2}(m+1)) \Gamma(\frac{1}{2}(n+2))}{4 \Gamma(\frac{1}{2}(m+n+3))} {}_3F_2\left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{m+1}{2} \\ 1, \frac{m+n+3}{2} \end{matrix} \middle| 1\right). \quad (6.9)$$

Using the obvious transformation $x \mapsto x'$, we have

$$\int_0^1 x^{2n+1} K(x)^a E(x)^b K'(x)^c E'(x)^d dx = \int_0^1 x(1-x^2)^n K'(x)^a E'(x)^b K(x)^c E(x)^d dx, \quad (6.10)$$

an equation which we appeal to often. Thus, using (6.10), we see that (6.8, 6.9) also encapsulate the moments for K' and E' . We note that for convergence, $m > -1, n > -2$. When $m = 1$ both formulas reduce to a ${}_2F_1$ and can be summed by Gauss' theorem (5.3).

If in addition $2m + n + 1 = 0$ in (6.8), then Dixon's theorem (14.14) applies and we may sum the ${}_3F_2$ explicitly in terms of the Γ function. For instance, we may compute $\int_0^1 K(x)/x' dx$ (which also follows from the Fourier series in Section

6.6). In (6.9), Dixon's theorem may only be applied to the single special case $\int_0^1 x' E(x) dx = \Gamma^4(1/4)/(48\pi)$.

In [40] (Chapter 5), the corresponding results for the moments of the generalised elliptic integrals are derived similarly.

Remark 6.2.1. It is also possible to work out, using the beta integral, a number of other results, such as

$$\int_0^1 x^m (1-x)^n K(x) dx = \frac{\pi \Gamma(m+1) \Gamma(n+1)}{2 \Gamma(m+n+2)} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{m+1}{2}, \frac{m+2}{2} \\ 1, \frac{m+n+2}{2}, \frac{m+n+3}{2} \end{matrix} \middle| 1 \right).$$

The above simplifies, for instance, when $m = n = -1/2$. ◇

6.3. Two complementary elliptic integrals

Though the simple cases corresponding to $n = 0$ in this section are tabulated in [66], the general results appear to be new.

In [207], Zudilin's Theorem connects, as a special case, triple integrals of rational functions over the unit cube with generalised hypergeometric functions ${}_7F_6$'s. We state a restricted form of the theorem which is sufficient for our purposes:

Theorem 6.1 (Zudilin). *Given h_0, \dots, h_5 for which both sides converge,*

$$\begin{aligned} & \int_{[0,1]^3} \frac{x^{h_2-1} y^{h_3-1} z^{h_4-1} (1-x)^{h_0-h_2-h_3} (1-y)^{h_0-h_3-h_4} (1-z)^{h_0-h_4-h_5}}{(1-x(1-y(1-z)))^{h_1}} dx dy dz \\ &= \frac{\Gamma(h_0+1) \prod_{j=2}^4 \Gamma(h_j) \prod_{j=1}^4 \Gamma(h_0+1-h_j-h_{j+1})}{\prod_{j=1}^5 \Gamma(h_0+1-h_j)} \times \\ & {}_7F_6 \left(\begin{matrix} h_0, 1 + \frac{h_0}{2}, h_1, h_2, h_3, h_4, h_5 \\ \frac{h_0}{2}, 1+h_0-h_1, 1+h_0-h_2, 1+h_0-h_3, 1+h_0-h_4, 1+h_0-h_5 \end{matrix} \middle| 1 \right). \end{aligned} \tag{6.11}$$

In Chapter 2, this theorem is used to derive hypergeometric evaluations for the moments of random walks from their triple integral representations.

The idea here is to write a single integral involving products of elliptic integrals as a double, then a triple integral of the required form, and then apply Theorem

6.1. To do so, we require the following formulas, which are readily verified [1]:

$$\int_0^1 \frac{dx}{\sqrt{x(1-x)(a-x)}} = \frac{2}{\sqrt{a}} K\left(\frac{1}{\sqrt{a}}\right), \quad (6.12)$$

$$\int_0^1 \sqrt{\frac{a-x}{x(1-x)}} dx = 2\sqrt{a} E\left(\frac{1}{\sqrt{a}}\right), \quad (6.13)$$

$$\int_a^1 \frac{dy}{\sqrt{y(1-y)(y-a)}} = 2K'(\sqrt{a}), \quad (6.14)$$

$$\int_a^1 \frac{\sqrt{y}}{\sqrt{(1-y)(y-a)}} dy = 2E'(\sqrt{a}). \quad (6.15)$$

Using the above relations, we have, for instance,

$$\begin{aligned} \int_0^1 E'(y)^2 dy &= \frac{1}{2} \int_0^1 \int_{a^2}^1 \sqrt{\frac{y}{(1-y)(y-a^2)}} E(\sqrt{1-a^2}) dy da \\ &= \frac{1}{4} \int_0^1 \int_0^1 \sqrt{\frac{y}{(1-y)z(1-z)}} E(\sqrt{1-yz}) dy dz \\ &= \frac{1}{8} \int_0^1 \int_0^1 \int_0^1 \sqrt{\frac{y(1-yz)}{(1-y)z(1-z)}} \sqrt{\frac{1}{1-yz} - x} dx dy dz \\ &= \frac{1}{8} \int_{[0,1]^3} \sqrt{\frac{y(1-x(1-y(1-z)))}{x(1-x)(1-y)z(1-z)}} dx dy dz. \end{aligned}$$

The first equality follows from (6.15), the second from changing $a^2 \mapsto yz$, the third from (6.13), and the fourth from $z \mapsto 1-z$. Now Theorem 6.1 applies to the last integral.

Similarly, by building up the E' integral then K' , we obtain:

$$\int_0^1 E'(x)K'(x) dx = \frac{1}{8} \int_{[0,1]^3} \sqrt{\frac{1-x(1-y(1-z))}{x(1-x)y(1-y)z(1-z)}} dx dy dz.$$

Alternatively, by building up the K' integral then E' , we get:

$$\int_0^1 E'(x)K'(x) dx = \frac{1}{8} \int_{[0,1]^3} \frac{\sqrt{y} dx dy dz}{\sqrt{x(1-x)(1-y)z(1-z)(1-x(1-y(1-z)))}}.$$

Finally, we also have

$$\int_0^1 K'(x)^2 dx = \frac{1}{8} \int_{[0,1]^3} \frac{dx dy dz}{\sqrt{x(1-x)y(1-y)z(1-z)(1-x(1-y(1-z)))}}.$$

Slightly generalising this strategy, we are led to:

Proposition 6.1. *For all real $n > -1$,*

$$(1) \quad \int_0^1 x^n E'(x)^2 dx = \frac{2^{4n}(n+1)^3(n+3)^2}{16(n+2)^3(n+4)} \frac{\Gamma^8\left(\frac{n+1}{2}\right)}{\Gamma^4(n+1)} {}_7F_6\left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{n+3}{2}, \frac{n+3}{2}, \frac{n+7}{4} \\ 1, \frac{n+3}{4}, \frac{n+2}{2}, \frac{n+4}{2}, \frac{n+4}{2}, \frac{n+6}{2} \end{matrix} \middle| 1\right), \quad (6.16)$$

$$(2) \quad \int_0^1 x^n E'(x)K'(x) dx = \frac{2^{4n}(n+1)^2}{16(n+2)} \frac{\Gamma^8\left(\frac{n+1}{2}\right)}{\Gamma^4(n+1)} {}_7F_6\left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{n+1}{2}, \frac{n+1}{2}, \frac{n+5}{4} \\ 1, \frac{n+1}{4}, \frac{n+2}{2}, \frac{n+2}{2}, \frac{n+2}{2}, \frac{n+4}{2} \end{matrix} \middle| 1\right) \\ = \frac{2^{4n}(n+1)^3(n+3)}{16(n+2)^3} \frac{\Gamma^8\left(\frac{n+1}{2}\right)}{\Gamma^4(n+1)} {}_7F_6\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{n+3}{2}, \frac{n+3}{2}, \frac{n+7}{4} \\ 1, \frac{n+3}{4}, \frac{n+2}{2}, \frac{n+4}{2}, \frac{n+4}{2}, \frac{n+4}{2} \end{matrix} \middle| 1\right), \quad (6.17)$$

$$(3) \quad \int_0^1 x^n K'(x)^2 dx = \frac{2^{4n}(n+1)}{16} \frac{\Gamma^8\left(\frac{n+1}{2}\right)}{\Gamma^4(n+1)} {}_7F_6\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{n+1}{2}, \frac{n+1}{2}, \frac{n+5}{4} \\ 1, \frac{n+1}{4}, \frac{n+2}{2}, \frac{n+2}{2}, \frac{n+2}{2}, \frac{n+2}{2} \end{matrix} \middle| 1\right). \quad (6.18)$$

When n is odd, the ${}_7F_6$'s reduce to known constants, which we prove below.

Theorem 6.2. *When n is odd, the n th moment of $K'^2, E'^2, K'E', K^2, E^2$ and KE is expressible as $a + b\zeta(3)$, where $a, b \in \mathbb{Q}$.*

PROOF. We prove the case for the pair K'^2 and K^2 ; the other two pairs are similar.

Firstly, when n is odd, the summand of the ${}_7F_6$ for K'^2 is a rational function:

$$\frac{(2k+m+1)(k+1)^2(k+2)^2 \cdots (k+m)^2}{(k+1/2)^4(k+3/2)^4 \cdots (k+m+1/2)^4}; \quad (6.19)$$

here we have ignored the rational constants at the front and wrote $n = 2m + 1$. We can explicitly sum (6.19) and verify the statement of the theorem for the first few moment of K'^2 . By using the change of variable $x \mapsto x'$ as in (6.10), we can likewise do this for K^2 .

Now it is not hard to show that the moments of K^2 satisfy a recursion:

$(n+1)^3 K_{n+2} - 2n(n^2+1)K_n + (n-1)^3 K_{n-2} = 2$. Results like this are proven in Section 6.8.2. The recursion shows that the statement holds for all odd moments of K^2 . Then (6.10) gives the result for K'^2 . \square

Remark 6.3.1. Note that by computing the moment of $E'(x)K'(x)$ in two ways, we obtain a transformation formula for the ${}_7F_6$'s involved. Also, by either one of

the two known transformations for non-terminating ${}_7F_6$'s [25, pp. 29 and 62], we can write each of our ${}_7F_6$ as the sum of two ${}_4F_3$'s, where one series readily simplifies to known constants when n is odd, while the harder term becomes reducible in light of Theorem 6.2. When n is even the reduction is more troublesome; after taking a limit, we have, for instance,

$$2 \int_0^1 K'(x)^2 dx = \sum_{k=0}^{\infty} \frac{\Gamma^4(k + \frac{1}{2})}{\Gamma^4(k + 1)} (H_k - H_{k-1/2}),$$

where H_n stands for the n th harmonic number; this result has already been recorded in Chapter 2. \diamond

Remark 6.3.2. Therefore, by Theorem 6.2, all the odd moments of $K'^2, E'^2, K'E'$ have particularly simple forms involving $\zeta(3)$. By using (6.10), we can iteratively obtain all the *odd moments* of K^2, E^2, KE . For example,

$$\int_0^1 x^3 K(x)^2 dx = \frac{1}{8}(2 + 7\zeta(3)), \quad \int_0^1 x K'(x)^2 dx = \frac{7}{4}\zeta(3).$$

\diamond

Remark 6.3.3. We sketch another proof of Theorem 6.2 by expanding (6.19) into partial fractions.

As each partial fraction has at most a quartic on the denominator, the irrational constants from the sum can only come from $\{\zeta(2), \zeta(3), \zeta(4)\}$, and possible contribution from the linear denominators. But as the linear terms must converge, their sum must eventually telescope, and hence contribute only a rational number.

We recall that partial fractions can be obtained via a derivative process akin to computing Taylor series coefficients; indeed, if we write

$$\frac{f(x)}{(x-a)^n} = \frac{A_1}{(x-a)} + \frac{A_2}{(x-a)^2} + \cdots + \frac{A_n}{(x-a)^n},$$

then $A_n = f(a), A_{n-1} = f'(a)/1!, \dots, A_1 = f^{(n-1)}(a)/(n-1)!$.

When applied to (6.19), it is easy to check that, when $n \equiv 3 \pmod{4}$, the presence of the numerator $2k + m + 1$ makes the terms with quadratic and quartic denominators telescope out, leaving us with rational numbers (these terms occur in pairs related by the transformation $k \mapsto -\frac{n+1}{2} - k$, where said linear numerator switches sign). Similarly, the terms with cubic denominators double.

When $n \equiv 1 \pmod{4}$, $2k + m + 1$ cancels out with one of the factors, making the corresponding denominator a cubic. We check that its partial fraction has no quadratic term: this is equivalent to showing (6.19) with all powers of $2k + m + 1$ removed has 0 derivative at $k = -\frac{n+1}{4}$, which holds as it is symmetric around that point. So in both cases only the cubic terms remain, giving us $\zeta(3)$.

This type of partial fraction argument is at the heart of the result that infinitely many odd zeta values are irrational (see [28], which, incidentally, is the motivation for Zudilin's Theorem 6.1).

Chronologically this was our first proof, after experimentally noticing that *Maple* was able to evaluate the relevant ${}_7F_6$'s without any trouble; upon increasing the `printlevel`, it became apparent that *Maple* was not using any transformations or summation formulas, so it was surmised that a more elementary method was used to evaluate the sum, i. e. partial fractions. \diamond

6.4. One elliptic integral and one complementary elliptic integral

Here we take advantage of the closed form for moments of K', E' which follow from (6.8) and (6.9):

$$\int_0^1 x^n K'(x) dx = \frac{\pi \Gamma^2(\frac{1}{2}(n+1))}{4 \Gamma^2(\frac{1}{2}(n+2))},$$

$$\int_0^1 x^n E'(x) dx = \frac{\pi \Gamma^2(\frac{1}{2}(n+3))}{2(n+1) \Gamma(\frac{1}{2}(n+2)) \Gamma(\frac{1}{2}(n+4))},$$

and the series for K, E equivalent to Definition 6.1:

$$K(x) = \sum_{k=0}^{\infty} \frac{\Gamma^2(k+1/2)}{\Gamma^2(k+1)} \frac{x^{2k}}{2}, \quad E(x) = \sum_{k=0}^{\infty} -\frac{\Gamma(k-1/2)\Gamma(k+1/2)}{\Gamma^2(k+1)} \frac{x^{2k}}{4}. \quad (6.20)$$

Hence, the proposition below may be simply proved by interchanging the order of summation and integration.

Proposition 6.2. *We have the following moments:*

(1)

$$\int_0^1 x^n K(x) K'(x) dx = \frac{\pi^2 \Gamma^2(\frac{1}{2}(n+1))}{8 \Gamma^2(\frac{1}{2}(n+2))} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{n+1}{2}, \frac{n+1}{2} \\ 1, \frac{n+2}{2}, \frac{n+2}{2} \end{matrix} \middle| 1 \right), \quad (6.21)$$

(2)

$$\int_0^1 x^n E(x) K'(x) dx = \frac{\pi^2 \Gamma^2(\frac{1}{2}(n+1))}{8 \Gamma^2(\frac{1}{2}(n+2))} {}_4F_3 \left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{n+1}{2}, \frac{n+1}{2} \\ 1, \frac{n+2}{2}, \frac{n+2}{2} \end{matrix} \middle| 1 \right), \quad (6.22)$$

(3)

$$\int_0^1 x^n K(x)E'(x) dx = \frac{\pi^2 (n+1)\Gamma^2(\frac{1}{2}(n+1))}{8 (n+2)\Gamma^2(\frac{1}{2}(n+2))} {}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{n+1}{2}, \frac{n+3}{2} \\ 1, \frac{n+2}{2}, \frac{n+4}{2} \end{matrix} \middle| 1\right), \quad (6.23)$$

(4)

$$\int_0^1 x^n E(x)E'(x) dx = \frac{\pi^2 (n+1)\Gamma^2(\frac{1}{2}(n+1))}{8 (n+2)\Gamma^2(\frac{1}{2}(n+2))} {}_4F_3\left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{n+1}{2}, \frac{n+3}{2} \\ 1, \frac{n+2}{2}, \frac{n+4}{2} \end{matrix} \middle| 1\right). \quad (6.24)$$

When n is odd, the moments yield a closed form as a rational multiple of π^3 plus a rational multiple of π , as we can expand the summand (a rational function) as partial fractions much like in Remark 6.3.3. To prove this observation, we need Legendre's relation [46]:

$$E(x)K'(x) + E'(x)K(x) - K(x)K'(x) = \frac{\pi}{2}. \quad (6.25)$$

Note that by using the symmetry between parts (2) and (3), as well as by applying (6.25), we obtain linear identities connecting these ${}_4F_3$'s. Due to the lack of Taylor expansions of E', K' around the origin as well as sufficiently simple moments for E, K , this method cannot be used to evaluate other moments.

Lemma 6.1. *For odd n , the n th moment of $K(x)K'(x)$ is a rational multiple of π^3 , and the n th moment of $E(x)K'(x), K(x)E'(x)$ and $E(x)E'(x)$ is $\frac{\pi}{4(n+1)}$ plus a rational multiple of π^3 .*

PROOF. We experimentally discover that, letting $g_n := \int_0^1 x^{2n-1} K(x)K'(x) dx$, we have the recursion

$$2n^3 g_{n+1} - (2n-1)(2n^2 - 2n + 1)g_n + 2(n-1)^3 g_{n-1} = 0.$$

This contiguous relation (see Chapter 14), once discovered, can be proven by extracting the summand, simplifying and summing using Gosper's algorithm. Thus, after computing two starting values, the claim is proven for the moments of KK' . Note that the recursion also holds when n is not an integer.

For the moments of EK' or KE' , we take the derivative of $x^{2n} K(x)K'(x)$ via the product rule, and integrate each piece in the result. By using (6.25) and the proven claim for the moments of KK' , we deduce that the term involving π is $\frac{\pi}{4(n+1)}$. For the moments of EE' , we instead consider the derivative of $(1-x^2)x^{2n} E(x)E'(x)$ and use the proven results for EK' and KE' . This trick involving integration by parts is exploited in Section 6.8. \square

Experimentally, we find that the sequence $h(n) := \pi^3 16^{n+1} g_{n+1}$ matches entry A036917 of the On-line Encyclopedia of Integer Sequences; indeed, they share the same recursion and initial values. Moreover, the OEIS provides

$$h(n) = \sum_{k=0}^n \binom{2n-2k}{n-k}^2 \binom{2k}{k}^2 = \frac{16^n \Gamma^2(n + \frac{1}{2})}{\pi \Gamma^2(n+1)} {}_4F_3 \left(\begin{matrix} -n, -n, \frac{1}{2}, \frac{1}{2} \\ \frac{1}{2} - n, \frac{1}{2} - n, 1 \end{matrix} \middle| 1 \right). \quad (6.26)$$

The first equality is routine as we can produce a recurrence for the binomial sum – for instance, using Sister Celine’s method; the second equality is notational. The sequence $h(n)$ will make another appearance in Chapter 12.

The generating function for $h(n)$ is simply

$$\sum_{n=0}^{\infty} h(n)t^n = \frac{4}{\pi^2} K(4\sqrt{t})^2,$$

which is again easy to prove using the series for $K(t)$. Recall that $h(n)$ is related to the moments of $K(x)K'(x)$, and thus we have:

Theorem 6.3.

$$\int_0^1 \frac{x}{1-t^2x^2} K(x)K'(x) dx = \frac{\pi}{4} K(t)^2. \quad (6.27)$$

Equation (6.27) seems to be a remarkable extension of its (much easier) cousins,

$$\int_0^1 \frac{1}{1-t^2x^2} K'(x) dx = \frac{\pi}{2} K(t) \quad \text{and} \quad \int_0^1 \frac{1}{1-t^2x^2} E'(x) dx = \frac{\pi}{2t^2} (K(t) - E(t)). \quad (6.28)$$

Manipulations of (6.27, 6.28) give myriads of integrals, we list some of them below (G denotes Catalan’s constant, investigated in Chapter 5):

$$\begin{aligned} \int_0^1 \frac{\arctan(x)}{x} K'(x) dx &= \pi G, \\ \int_0^1 \frac{2}{x} K(x)K'(x)(K(x) - E(x)) dx &= \int_0^1 K(x)^2 E'(x) dx, \\ \int_0^1 {}_2F_1 \left(\begin{matrix} 1, \frac{n+1}{2} \\ \frac{n+3}{2} \end{matrix} \middle| x^2 \right) x K(x)K'(x) dx &= \frac{(n+1)\pi}{4} \int_0^1 t^n K(t)^2 dt. \end{aligned}$$

The last identity specialises to

$$\int_0^1 \frac{-\log(1-x^2)}{x} K(x)K'(x) dx = \frac{7}{8} \pi \zeta(3), \quad (6.29)$$

while it is possible to similarly find

$$\int_0^1 \frac{-\log(1-x^2)}{x} K(x)E'(x) dx = \frac{\pi^3}{12}.$$

By setting $t = i$ in (6.27) (this also works for (6.28)) and appealing to (6.33), we obtain

$$\int_0^1 \frac{xK(x)K'(x)}{1+x^2} dx = \frac{\Gamma^4(\frac{1}{4})}{128}. \quad (6.30)$$

6.5. Sporadic results

We list some results found by ad hoc methods; some are not moment evaluations per se, while others are preparatory for later sections.

6.5.1. Explicit primitives. Curiously, a small number of integrals happen to have explicit primitives; we list some here:

$$x^n K(x), x^n E(x), \frac{x^n E(x)}{1-x^2}, \frac{E(x)}{1 \pm x} \text{ and } \frac{x F(x)}{(1-x^2)^{3/2}},$$

where F can be K, K', E or E' . The primitives are expressible in terms of K and E when $n > 0$ is odd or when $n < 0$ is even in the first three cases (and also when $n = 0$ in the third case). Moreover, $(E(x) - K(x))/x$ has a primitive (being $E(x)$).

The last case, and many other integrals, are found in [101]. We sample two other integrals from [101] to show the flavour of the identities therein:

$$\int_0^1 \frac{x K(x)}{(1-z^2 x^2)x'} dx = \frac{\pi}{2z'} K(z),$$

proven by $x \mapsto x'$, and

$$\int_0^1 x P_n(1-2x^2) K(x) dx = \frac{(-1)^n}{(2n+1)^2},$$

which involves the Legendre polynomials.

Trivially, transformations of the above list still yield explicit primitives. We note that some computer algebra systems, when used naïvely, struggle to find primitives which come from this very short list, one example is given by applying $x \mapsto x'$ in the last case:

$$\int \frac{K'(x)}{x^2} dx = \frac{E'(x) - K'(x)}{x}.$$

These cases also give rise to interesting definite integrals, we only record a couple here:

$$\int_0^1 \frac{E'(x) - 1}{x} dx = 2 \log 2 - 1, \quad \int_0^1 \frac{E'(x) - 1}{x^2} dx = 1. \quad (6.31)$$

A more thorough investigation is undertaken in Chapter 7.

6.5.2. Imaginary argument. In [1] vol III, some integrals with the argument ix are considered, e. g.

$$\int_0^1 xK'(x)K(ix) dx = \frac{1}{2}G\pi.$$

This can be proven by expanding $xK(ix)$ as a series and summing the moments of $K'(x)$. Other evaluations are done similarly; for instance, we can easily obtain recursions for the moments of $K(ix)$ and $E(ix)$.

We also record here that Euler's hypergeometric transformation [11]

$${}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix} \middle| z\right) = (1-z)^{-a} {}_2F_1\left(\begin{matrix} a, c-b \\ c \end{matrix} \middle| \frac{z}{z-1}\right) \quad (6.32)$$

gives

$$E(ix) = \sqrt{x^2+1} E(x/\sqrt{x^2+1}), \quad K(ix) = 1/\sqrt{x^2+1} K(x/\sqrt{x^2+1}). \quad (6.33)$$

6.5.3. Quadratic transforms. Using the quadratic transforms (6.4, 6.5), we obtain

$$\begin{aligned} \int_0^1 K(x)^n dx &= \frac{1}{2} \int_0^1 K'(t)^n \left(\frac{1+t}{2}\right)^{n-2} dt, \\ \int_0^1 K'(x)^n dx &= 2 \int_0^1 K(t)^n (1+t)^{n-2} dt. \end{aligned} \quad (6.34)$$

Setting $n = 1$ we recover the known special case

$$\int_0^1 \frac{K(x)}{x+1} dx = \frac{\pi^2}{8}.$$

Using a cubic transform of the Borweins [45], this identity is generalised in Chapter 5. The appropriate generalisation of (6.3) – itself obtained by setting $n = 2$ in (6.34) – is

$$\int_0^1 {}_2F_1\left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| 1-x^3\right)^2 dx = 3 \int_0^1 {}_2F_1\left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| x^3\right)^2 dx.$$

Using (6.5) on the integrand $xK(x)^3$, we get

$$\int_0^1 2(1-x)K(x)^3 dx = \int_0^1 xK(x)^3 dx,$$

when combined with (6.34), we deduce

$$\int_0^1 K'(x)^3 dx = \frac{10}{3} \int_0^1 K(x)^3 dx = 5 \int_0^1 xK(x)^3 dx = 5 \int_0^1 xK'(x)^3 dx. \quad (6.35)$$

Using (6.6, 6.7), we have

$$\int_0^1 E(x)^n \frac{2^{n+1}}{(x+1)^{n+2}} dx = \int_0^1 (E'(x) + xK'(x))^n dx, \quad (6.36)$$

$$\int_0^1 E'(x)^n \frac{2^{n+1}}{(x+1)^{n+2}} dx = \int_0^1 (2E(x) - (1-x^2)K(x))^n dx. \quad (6.37)$$

When $n = 1, 2$ we obtain closed forms, such as

$$\int_0^1 \frac{E(x)}{(x+1)^3} dx = \frac{\pi^2}{32} + \frac{1}{4}, \quad \int_0^1 \frac{E'(x)}{(x+1)^3} dx = \frac{G}{8} + \frac{5}{16}.$$

6.5.4. Relationship to random walks. In Chapter 2, many moment relations are derived while computing $W_4(n)$, the n th moment of the distance from the origin of a 4-step uniform random walk on the plane. For instance, we have:

$$W_4(1) = \frac{16}{\pi^3} \int_0^1 (1-3x^2)K'(x)^2 dx.$$

In [57] (Chapter 3) and [20, formula (89)], the following identities are given via Meijer G-functions:

$$\begin{aligned} \frac{\pi^3}{4} W_4(-1) &= \int_0^{\pi/2} K(\sin t)^2 \sin t dt = 2 \int_0^{\pi/2} K(\sin t)^2 \cos t dt \\ &= \int_0^{\pi/2} K(\sin t)K(\cos t) dt = 2 \int_0^{\pi/2} K(\sin t)K(\cos t) \cos^2 t dt. \end{aligned} \quad (6.38)$$

The last equality follows from the general identity (proven by $x \mapsto x'$)

$$\int_0^1 2F(x^2)F(1-x^2)\sqrt{1-x^2} dx = \int_0^1 F(x^2)F(1-x^2) \frac{dx}{\sqrt{1-x^2}}.$$

6.6. Fourier series

As recorded in [20], we have the following Fourier (sine) series valid on $(0, \pi)$:

Lemma 6.2.

$$K(\sin t) = \sum_{n=0}^{\infty} \frac{\Gamma^2(n+1/2)}{\Gamma^2(n+1)} \sin((4n+1)t). \quad (6.39)$$

For completeness, we sketch a proof here:

PROOF. By symmetry we see that only the coefficients of $\sin((2n+1)t)$ are non-zero. Indeed, by a change of variable $\cos t \mapsto x$, the coefficients are

$$\frac{4}{\pi} \int_0^1 K'(x) \frac{\sin((2n+1)t)}{\sin t} dt.$$

The fraction in the integrand is precisely $U_{2n}(x)$, where $U_n(x)$ denotes the *Chebyshev polynomial of the second kind*, given by

$$U_{2n}(x) = \sum_{k=0}^n (-1)^k \binom{2n-k}{k} (2x)^{2n-2k}.$$

We now interchange summation and integration, and use the moments of K' . The resulting coefficient contains a ${}_3F_2$, which after a transformation [25, section 3.2] becomes amenable to Saalschütz's theorem (14.10), and we obtain (6.39). \square

The same method gives a Fourier sine series for $E(\sin t)$ valid on $(0, \pi)$, which we have not been able to locate in the literature. In mirroring the last step, the resulting ${}_3F_2$ is reduced to the closed form below using Sister Celine's method:

Lemma 6.3.

$$E(\sin t) = \sum_{n=0}^{\infty} \frac{\Gamma^2(n+1/2)}{2\Gamma^2(n+1)} \sin((4n+1)t) + \sum_{n=0}^{\infty} \frac{(n+1/2)\Gamma^2(n+1/2)}{2(n+1)\Gamma^2(n+1)} \sin((4n+3)t). \quad (6.40)$$

Parseval's formula [125, p. 156] applied to (6.39) and (6.40) gives

$$\begin{aligned} \int_0^{\pi/2} K(\sin t)^2 dt &= 2 \int_0^{\pi/2} K(\sin t)E(\sin t) dt \\ &= \int_0^1 \frac{K(x)^2}{\sqrt{1-x^2}} dx = \int_0^1 \frac{K'(x)^2}{\sqrt{1-x^2}} dx = \int_0^1 \frac{1+x}{\sqrt{x}} K(x)^2 dx \\ &= 2 \int_0^1 \frac{K(x)E(x)}{\sqrt{1-x^2}} dx = 2 \int_0^1 K(x)K'(x) dx = \frac{\pi^3}{4} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle| 1 \right). \end{aligned} \quad (6.41)$$

We also get $\int_0^{\pi/2} K(\sin t)^2 \cos(4t) dt$ as a sum of three ${}_4F_3$'s, and $\int_0^{\pi/2} E(\sin t)^2 dt$ as a sum of four ${}_4F_3$'s. Section 3.7 of [20] provides a number of identities of this sort with more exotic arguments, as well as connections with Meijer G-functions.

Experimentally we find the surprisingly simple answer to the integral

$$\begin{aligned} \int_0^{\pi/2} K(\sin t)^2 \frac{\sin 4t}{4} dt &= \int_0^1 K(x)^2 (x - 2x^3) dx = \int_0^1 xK(x)(x^2K(x) - E(x)) dx \\ &= \int_0^1 K'(x)^2 (2x^3 - x) dx = \int_0^1 xK'(x)(x^2K'(x) - E'(x)) dx \\ &= \int_0^1 xK^2(x) - 2xE(x)K(x) dx = -\frac{1}{2}. \end{aligned} \quad (6.42)$$

All equalities are routine to check except for the last one, which is equivalent to

$$\int_0^1 xK(x)^2 + 2xE(x)^2 - 3xK(x)E(x) dx = 0,$$

and so the equality holds as we know all the odd moments.

Inserting a factor of $\cos^2 t$ before squaring the Fourier series (6.39) and integrating, we are led to

$$\int_0^1 x' K(x)^2 dx = \frac{\pi^3}{16} \left({}_2F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle| 1 \right) - 1 \right) = \int_0^1 \frac{\sqrt{x}}{x+1} K'(x)^2 dx. \quad (6.43)$$

Subtracting (6.43) from (6.41) gives

$$\begin{aligned} \int_0^1 x' K'(x)^2 dx &= \int_0^1 \frac{x^2}{x'} K(x)^2 dx = \int_0^1 \frac{4\sqrt{x}}{x+1} K(x)^2 dx \\ &= \frac{\pi^3}{16} \left({}_2F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle| 1 \right) + 1 \right). \end{aligned} \quad (6.44)$$

The Fourier series (6.39) combined with a quadratic transform gives:

$$\begin{aligned} \int_0^{\pi/2} K(\sin t) dt &= \int_0^1 \frac{K(x)}{\sqrt{1-x^2}} dx = \int_0^1 \frac{K'(x)}{\sqrt{1-x^2}} dx = \int_0^1 \frac{K(x)}{\sqrt{x}} dx \\ &= \frac{1}{2} \int_0^1 \frac{K'(x)}{\sqrt{x}} dx = K \left(\frac{1}{\sqrt{2}} \right)^2 = \frac{1}{16\pi} \Gamma^4 \left(\frac{1}{4} \right). \end{aligned} \quad (6.45)$$

A generalisation of this result is found in Chapter 5.

Finally, we give a more exotic example: using the Fourier series expansion of $\cos(t)K(\sin(t))K(\sin(2t))$, we get

$$\int_0^1 K(x)K(2xx') dx = \frac{\pi^3}{8} {}_4F_3 \left(\begin{matrix} \frac{1}{4}, \frac{1}{4}, \frac{3}{4}, \frac{3}{4} \\ 1, 1, 1 \end{matrix} \middle| 1 \right).$$

6.7. Legendre's relation

Legendre's relation $EK' + E'K - KK' = \frac{\pi}{2}$ is related to the Wronskian of K and E , and shows that the two integrals are closely coupled (we have already seen its role in the proof of Lemma 6.1).

If we multiply both sides of Legendre's relation (6.25) by $K'(x)$ and integrate, we arrive at

$$\int_0^1 3E'(x)K'(x)K(x) - K(x)K'(x)^2 dx = \frac{\pi^3}{8}. \quad (6.46)$$

Similarly, had we multiplied by $K(x)$, the result would be

$$\begin{aligned} &\int_0^1 3E(x)K(x)K'(x) - 2K(x)^2K'(x) dx \\ &= \int_0^1 2E'(x)K(x)^2 - E(x)K(x)K'(x) dx = \pi G. \end{aligned} \quad (6.47)$$

Using closed forms of the moments, we also have:

$$\int_0^1 2xE'(x)K(x)^2K'(x) - xK(x)^2K'(x)^2 dx = \frac{\pi^4}{32},$$

$$\int_0^1 2xE'(x)^2K(x)E(x) - xK(x)K'(x)E(x)E'(x) dx = \frac{\pi^2}{16} + \frac{\pi^4}{128}.$$

Of course, we can multiply Legendre's relation by any function whose integral vanishes on the interval $(0, 1)$ to produce another relation. Suitable candidates for the function include $x(K(x) - K'(x))$, $x(2K'(x) - 3E'(x))$, $2E'(x) - K'(x)$, $2E(x) - K(x) - 1$, and a vast range of polynomials. For instance one could obtain

$$\int_0^1 2E'^2(x)K(x) + 2E(x)E'(x)K'(x) - 5E'(x)K(x)K'(x) + K(x)K'(x)^2 dx = 0.$$

It seems difficult to 'uncouple' any of the above sums and differences to obtain a closed form for the integral of a single product, without the results in Conjecture 6.2. However, (6.46), (6.47) do yield closed forms as we later prove that conjecture – these results will be made clear in Chapter 7.

6.8. Integration by parts

The following simple but fruitful idea is crucial to this section. We look at the derivative $(1-x^2)^n \frac{d}{dx} (x^k K(x)^a E(x)^b K'(x)^c E'(x)^d)$ (the formulas for the derivatives of E and K can be found in Section 5.1), and integrate by parts to yield

$$\int_0^1 (1-x^2)^n \frac{d}{dx} (x^k K(x)^a E(x)^b K'(x)^c E'(x)^d) dx$$

$$= \int_0^1 2nx(1-x^2)^{n-1} x^k K(x)^a E(x)^b K'(x)^c E'(x)^d dx + C, \quad (6.48)$$

where the constant $C \neq 0$ if and only if the integrand is a power of E or E' .

In practice, we take $n, k \in \{0, 1, 2\}$ to produce the cleanest identities. We also explore the cases when n is a half-integer, as well as replacing $1-x^2$ by $1-x$ in (6.48).

6.8.1. Bailey's tables for products of two elliptic integrals. We now systematically analyse the tables kindly provided by D. H. Bailey, the construction of which is described in [19]. The tables contain all known (in fact, probably *all*) linear relations for integrals of products of up to k elliptic integrals ($k \leq 6$) and a polynomial in x with degree at most 5. In this subsection we exclusively look at the case $k = 2$ and spell out the details.

We use $x \frac{d}{dx} E(x)^2 = 2E(x)^2 - 2E(x)K(x)$ and integrate by parts to deduce

$$\int_0^1 3E(x)^2 - 2E(x)K(x) dx = 1. \quad (6.49)$$

More generally,

$$1 = (n + k + 1) \int_0^1 x^k E(x)^n - nx^k E(x)^{n-1} K(x) dx. \quad (6.50)$$

Two more special cases of the above are prominent:

$$\int_0^1 5x^2 E(x)^2 - 2x^2 E(x)K(x) dx = 1, \quad (6.51)$$

$$\int_0^1 (n + 2)x^{n-1} E(x)^2 - 2x^{n-1} E(x)K(x) dx = 1. \quad (6.52)$$

The derivative of $K(x)E(x)$ (via integration by parts) gives

$$\int_0^1 (1 - 3x^2)E(x)K(x) + E(x)^2 - (1 - x^2)K(x)^2 dx = 0, \quad (6.53)$$

which is part of the more general

$$\begin{aligned} \int_0^1 nx^{n-1} E(x)K(x) - (n + 2)x^{n+1} E(x)K(x) + x^{n-1} E(x)^2 \\ - x^{n-1} K(x)^2 + x^{n+1} K(x)^2 dx = 0. \end{aligned} \quad (6.54)$$

The derivative of $K(x)^2$ produces

$$\int_0^1 (1 + x^2)K^2(x) dx = 2 \int_0^1 K(x)E(x) dx, \quad (6.55)$$

while more generally,

$$\int_0^1 2x^{n-1} E(x)K(x) + (n - 2)x^{n-1} K(x)^2 - nx^{n+1} K(x)^2 dx = 0. \quad (6.56)$$

The derivative of $E'(x)^2$ gives (using (6.10) for the first equality)

$$\int_0^1 2xE'(x)^2 - xE'(x)K'(x) dx = \int_0^1 2xE(x)^2 - xE(x)K(x) dx = \frac{1}{2}.$$

The derivative of $K'(x)^2$ gives

$$\int_0^1 2K'(x)E'(x) - (1 - x^2)K'(x)^2 dx = 0, \quad (6.57)$$

re-confirming a result from Chapter 2, which is first proven in a much more round-about way via a non-trivial group action on the integrand.

The derivative of $E'(x)K'(x)$ gives

$$\int_0^1 (1 - 3x^2)E'(x)K'(x) dx = \int_0^1 E'(x)^2 - x^2 K'(x)^2 dx,$$

which, when combined with our last result, gives

$$\int_0^1 (1 + 3x^2)E'(x)K'(x) dx = \int_0^1 K'(x)^2 - E'(x)^2 dx.$$

The derivative of $K(x)K'(x)$ gives

$$\int_0^1 x^2 K(x)K'(x) + K(x)E'(x) - K'(x)E(x) dx = 0,$$

which, when combined with Legendre's relation (6.25), results in

$$\int_0^1 2E'(x)K(x) - (1 - x^2)K(x)K'(x) dx = \frac{\pi}{2}.$$

Our results here and in previous sections actually provide direct proofs of most entries in Bailey's tables where the polynomial is linear. In fact, it would simply be a matter of tenacity to prove many entries involving polynomial of higher degrees. As an example, we indicate how to prove an entry which requires more work:

$$\int_0^1 E(x)(3E'(x) - K'(x)) dx = \frac{\pi}{2}. \quad (6.58)$$

We write the left hand side as two ${}_4F_3$'s, combine their summands into a single term and simplify; the result can be summed explicitly by Gosper's algorithm, and the limit on the right hand side follows.

The same method applies to other entries, e. g.

$$\begin{aligned} \int_0^1 E'(x)K(x) - E(x)K'(x) + x^2 K(x)K'(x) dx &= 0, \\ \int_0^1 K'(x)^2 - 4E'(x)K'(x) + 3E'(x)^2 dx &= 0. \end{aligned}$$

There is only one entry in Bailey's tables (for linear polynomials) that we cannot prove in this chapter, though it is true to at least 1500 digits:

Conjecture 6.1.

$$\int_0^1 2K(x)^2 - 4E(x)K(x) + 3E(x)^2 - K'(x)E'(x) dx \stackrel{?[1]}{=} 0. \quad (6.59)$$

(The notation $\stackrel{?[k]}{=}$ denotes the equivalence of conjectural identities, where all equations with the same k are equivalent as conjectures.)

We note that, among moments of products of two elliptic integrals, there are only five that we cannot find closed forms for in this chapter:

$$E(x)^2, x^2 E(x)^2, E(x)K(x), x^2 E(x)K(x), x^2 K(x)^2,$$

as all the odd moments are known, and the other even moments may be obtained from these ignition values. In this chapter we can only prove four equations connecting them, namely (6.49, 6.51, 6.53, 6.55). A proof of (6.59) would give us enough information to solve for all five moments; for instance, we would have

$$\frac{32}{\pi^4} \int_0^1 E(x)K(x) dx \stackrel{?[1]}{=} \frac{16}{\pi^4} {}_7F_6 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{5}{4} \\ \frac{1}{4}, 1, 1, 1, 1, 1 \end{matrix} \middle| 1 \right) - \frac{1}{2} {}_7F_6 \left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{5}{4} \\ \frac{1}{4}, 1, 1, 1, 1, 2 \end{matrix} \middle| 1 \right).$$

This is resolved in Chapter 7.

6.8.2. Recurrences for the moments. As already hinted in the proof of Lemma 6.1, the moments enjoy recurrences with polynomial coefficients. For example, by combining (6.52, 6.54, 6.56), we obtain, with $K_n := \int_0^1 x^n K(x)^2 dx$,

$$(n+1)^3 K_{n+2} - 2n(n^2+1)K_n + (n-1)^3 K_{n-2} = 2. \quad (6.60)$$

This shows that K_n is a rational number plus a rational multiple of $\zeta(3)$ for odd n , as this approach is used in the proof of Theorem 6.2.

Similarly, recurrences for other products may be obtained, though the linear algebra becomes more prohibitive. We have, for $E_n := \int_0^1 x^n E(x)^2 dx$,

$$(n+1)(n+3)(n+5)E_{n+2} - 2(n^3+3n^2+n+1)E_n + (n-1)^3 E_{n-2} = 8, \quad (6.61)$$

while the recursion for the moments of EK follows from this and (6.52). The recursion for the moments of K'^2 , and, amazingly, for KK' , are identical to (6.60) except the right hand side is 0. Moreover, the $\zeta(3)$ parts in the odd moments of K'^2 and K^2 are *equal*, and satisfy the same recursion (with proportional initial conditions) as the odd moments of KK' .

6.8.3. More results. We discover some results not found in Bailey's tables by incorporating constants such as π and G into the search space. Below we highlight some of the prettier formulas.

Taking $(1-x^2)\frac{d}{dx}(x^2K(x)^2)$ and integrating by parts, we obtain

$$\int_0^1 xK(x)K'(x) dx = \int_0^1 2x^3K(x)K'(x) dx = \int_0^1 \frac{1-x}{1+x} K(x)K'(x) dx = \frac{\pi^3}{16}. \quad (6.62)$$

The derivative of $x^{2n}K(x)K'(x)$ together with (6.25) gives

$$\int_0^1 x^{2n-1}(E'(x)K(x) + n(x^2-1)K(x)K'(x)) dx = \frac{\pi}{8n}. \quad (6.63)$$

We can take $n = \frac{1}{2}$ in (6.48); for instance, the derivative of $xx'K(x)$ gives

$$\int_0^1 \frac{E(x)}{x'} dx = \int_0^1 \frac{x^2 K(x)}{x'} dx,$$

while the derivative of $xx'K(x)^2$ recaptures (6.41).

The derivative of $x'K(x)$ gives

$$\int_0^1 \frac{K(x) - E(x)}{xx'} dx = \frac{\pi}{2},$$

note that each part does not converge. In fact,

$$K(x) - E(x) = \frac{\pi x^2}{4} {}_2F_1\left(\frac{1}{2}, \frac{3}{2} \middle| x^2\right), \quad (6.64)$$

therefore for example

$$\int_0^1 \frac{K(x) - E(x)}{x} dx = \frac{\pi}{2} - 1, \quad \int_0^1 \frac{K(x) - E(x)}{x^2} dx = 1, \quad \int_0^1 \frac{K(x) - E(x)}{xx'} dx = \frac{\pi}{2}.$$

The general case is

$$\int_0^1 x^m x'^n (K(x) - E(x)) dx = \frac{\pi \Gamma(\frac{3+m}{2}) \Gamma(\frac{2+n}{2})}{8 \Gamma(\frac{5+m+n}{2})} {}_3F_2\left(\frac{1}{2}, \frac{3}{2}, \frac{3+m}{2} \middle| 1\right).$$

The derivative of $xE(x)$ gives

$$2E(x) - K(x) = \frac{\pi}{2} {}_2F_1\left(-\frac{1}{2}, \frac{3}{2} \middle| x^2\right),$$

so for instance

$$\int_0^1 xx'(2E(x) - K(x)) dx = \frac{\pi^2}{32},$$

and the general case is

$$\int_0^1 x^m x'^n (2E(x) - K(x)) dx = \frac{\pi \Gamma(\frac{1+m}{2}) \Gamma(\frac{2+n}{2})}{4 \Gamma(\frac{3+m+n}{2})} {}_3F_2\left(-\frac{1}{2}, \frac{3}{2}, \frac{1+m}{2} \middle| 1\right).$$

We can clearly analyse a number of other ${}_2F_1$'s this way.

The derivative of $x(1-x)K(x)^2$ gives

$$\int_0^1 \frac{2K(x)E(x)}{x+1} dx = \int_0^1 K(x)^2 dx.$$

Collecting what we know about the integral of $K(x)^2$, we have the following:

Theorem 6.4. *The alternative forms of equation (6.3) are:*

$$\begin{aligned}
 \int_0^1 K(x)^2 dx &= \frac{1}{2} \int_0^1 K'(x)^2 dx = \int_0^1 K'(x)^2 \frac{x}{x'} dx \\
 &= \int_0^1 K(x)K'(x)x' dx = \frac{1}{2} \int_0^1 K(x)K'(x) \frac{dx}{x'} \\
 &= \int_0^1 \frac{(1+x)K(x)K'(x)}{4\sqrt{x}} dx = \int_0^1 \frac{2\sqrt{x}K(x)K'(x)}{1+x} dx \\
 &= \int_0^1 \frac{(1-x)K'(x)^2}{8\sqrt{x}} dx = \int_0^1 \frac{(1-x)K(x)^2}{\sqrt{x}} dx \\
 &= \int_0^1 \frac{2K(x)E(x)}{x+1} dx \\
 &= \frac{2}{\pi} \int_0^1 \frac{\arcsin x}{\sqrt{1-x^2}} K(x)K'(x) dx = \frac{4}{\pi} \int_0^1 \operatorname{arctanh}(x)K(x)K'(x) dx.
 \end{aligned}$$

PROOF. The last two equalities follow from (6.27); the rest has been proven elsewhere (e. g. use (6.38), and the quadratic transformations). \square

Note that the first integral in the third line above breaks up into two moments of KK' , thus we can decompose the ${}_7F_6$ this way:

$$\int_0^1 K(x)^2 dx = \frac{\Gamma^4(\frac{1}{4})}{64} {}_4F_3\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}, \frac{1}{2} \mid 1\right) + \frac{\pi^4}{\Gamma^4(\frac{1}{4})} {}_4F_3\left(\frac{1}{2}, \frac{1}{2}, \frac{3}{4}, \frac{3}{4} \mid 1\right). \quad (6.65)$$

6.8.4. Bailey's tables for products of three elliptic integrals. We now consider the linear relations involving the product of three elliptic integrals ($k = 3$ in the tables). As the number of relations found is huge, we restrict most of our attention to a class of integrals that turns out to be pair-wise related by a rational factor.

Below we tabulate all the products for which 'neat' integrals may be deduced by differentiating them and integrating by parts:

Product:	Integral:
$K(x)^3$	$\int_0^1 2K(x)^3 - 3K(x)^2E(x) dx = 0$
$K(x)^2K'(x)$	$\int_0^1 K(x)^2E'(x) + K(x)^2K'(x) - 2K(x)K'(x)E(x) dx = 0$
$K'(x)^2K(x)$	$\int_0^1 E(x)K'(x)^2 - 2E'(x)K(x)K'(x) dx = 0$
$K'(x)^3$	$\int_0^1 K'(x)^3 - 3K'(x)^2E'(x) dx = 0$
$E'(x)^3$	$\int_0^1 5xE'(x)^3 - 3xE'(x)^2K'(x) dx = 1$
$E(x)^3$	$\int_0^1 4E(x)^3 - 3E(x)^2K(x) dx = 1$

We can prove

$$\int_0^1 K(x)^2 K'(x) dx = \frac{2}{3} \int_0^1 K(x) K'(x)^2 dx,$$

by making the change of variable $x \mapsto \frac{1-x}{1+x}$ to the left hand side and using the quadratic transform (6.4). The integral splits into two pieces; we apply $x \mapsto \frac{2\sqrt{x}}{1+x}$ to one piece followed by another quadratic transform (6.5). We obtain

$$\int_0^1 3xK(x)K'(x)^2 dx = \int_0^1 K(x)K'(x)^2 dx;$$

finally the claim is proven by combining the pieces.

If we make the change of variable $x \mapsto \frac{1-x}{1+x}$, then apply (6.6), we have

$$\int_0^1 \frac{K(x)^2 E(x)}{1+x} dx = \frac{4}{9} \int_0^1 K(x)^3 dx.$$

Integrating $x^2(1-x)K(x)^3$ by parts, we can show that $\int_0^1 xK(x)^2 E(x)/(x+1) dx$ is also linearly related to the above integral.

Therefore, gathering the results in this section and equation (6.35), we have determined:

Theorem 6.5. *Any two integrals in each of the following two groups are related by a rational factor:*

$$K(x)^3, K'(x)^3, xK(x)^3, xK'(x)^3, K(x)^2 E(x), K'(x)^2 E'(x), \frac{K^2(x)E(x)}{1+x}, \frac{xK^2(x)E(x)}{1+x};$$

$$K(x)K'(x)^2, K(x)^2 K'(x), xK(x)K'(x)^2, xK(x)^2 K'(x). \quad (6.66)$$

From the results in this chapter, we cannot yet show that any two integrals, one from each group, are related by a rational factor, though this is resolved in Chapter 7. In fact, the Inverse Symbolic Calculator gives the remarkable evaluation:

Conjecture 6.2.

$$\int_0^1 K'(x)^3 dx \stackrel{?[2]}{=} 2K\left(\frac{1}{\sqrt{2}}\right)^4 = \frac{\Gamma^8(\frac{1}{4})}{128\pi^2}. \quad (6.67)$$

Once proven, this would give explicit closed forms for the integrals of $E'K'K$, $EK'K$, and $E'K^2$ by the results of Section 6.7.

In view of Theorem 6.5, (6.21) and (6.26), interchanging the order of summation and integration gives an equivalent form of Conjecture 6.2:

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{8}{(2n+1)^2} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, n+1, n+1 \\ 1, n+\frac{3}{2}, n+\frac{3}{2} \end{matrix} \middle| 1 \right) \\ &= \sum_{n=0}^{\infty} \frac{\Gamma^4(n+\frac{1}{2})}{\Gamma^4(n+1)} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, -n, -n \\ 1, \frac{1}{2}-n, \frac{1}{2}-n \end{matrix} \middle| 1 \right) \stackrel{?[2]}{=} \frac{\Gamma^8(\frac{1}{4})}{24\pi^4}. \end{aligned} \quad (6.68)$$

In fact, the integral in Conjecture 6.2 has re-expressions as integrals over products of theta, or of Dedekind η functions. These alternative forms make the conjecture easier to attack, and we prove the conjecture in Section 7.9.

6.8.5. Products of four elliptic integrals and conclusion. If we take the derivative of $K(x)^4$, use the integral (6.34) connecting $K'(x)^4$ and $K(x)^4$, plus a quadratic transform, then we obtain

$$\int_0^1 24E(x)K(x)^3 - 8K(x)^4 - K'(x)^4 dx = 0, \quad (6.69)$$

which is one of the first non-trivial identities in Bailey's tables for $k = 4$. Many more tabulated relations for products of three and four elliptic integrals can be proven, albeit the complexity of the proofs increases. As perceptively noted in [19],

“[it] seems to be more and more the case as experimental computational tools improve, our ability to discover outstrips our ability to prove.”

CHAPTER 7

More Integrals of K and E

ABSTRACT. We study integrals of elliptic integrals more closely. In particular, it transpires that more fruitful relations can be seen by looking at integrals of the form $\int_0^1 F(x)(1+x)^n dx$ than by looking at the raw moments. Using this line of inquiry, as well as other new ideas, we resolve all the conjectures in Chapter 6.

7.1. One elliptic and one complementary elliptic integral

In this section we take a close look at integrals containing the product of an elliptic integral with a complementary elliptic integral. Let A denote $\int_0^1 K(x)K'(x) dx$ and B denote $\int_0^1 x^2 K(x)K'(x) dx$. Integration by parts (see Chapter 6) gives

$$2 \int_0^1 K(x)E'(x) dx = \frac{\pi}{2} + A - B,$$

which we implicitly use in the rest of this section.

Example 7.1.1 (Starting values). Our first goal is to find, in terms of A and B , evaluations of $\int_0^1 G(x)H'(x)/(1+x)^l dx$, where $G, H \in \{E, K\}$, and $l \in \{1, 2\}$. The details are given below.

Integrating $x(1-x)K'(x)K(x)$ by parts, we arrive at

$$A = \int_0^1 \frac{E(x)K'(x) - K(x)E'(x) + K(x)K'(x)}{1+x} dx,$$

which, when combined with Legendre's relation (6.25), gives

$$\int_0^1 \frac{E(x)K'(x)}{1+x} dx = \frac{A}{2} + \frac{\pi}{4} \log 2. \tag{7.1}$$

Similarly, integrating $x(1-x)K(x)E'(x)$ by parts, we obtain

$$\begin{aligned} & \int_0^1 2xK(x)E'(x) - xK(x)K'(x) dx + (A - B) \\ &= \int_0^1 \frac{E(x)E'(x) - K(x)E'(x) + K(x)K'(x)}{1+x} dx, \end{aligned}$$

but as all the odd moments are known (Chapter 6), the left hand side reduces to $\pi/4 + A - B$. Combining this result with Legendre's relation and (7.1), we get

$$\int_0^1 \frac{E(x)E'(x)}{1+x} dx = \frac{B}{2} + \frac{\pi}{4} \log 2. \quad (7.2)$$

Let $x \mapsto (1-x)/(1+x)$ in the integrand $K(x)K'(x)/(1+x)$. Applying both quadratic transforms (6.4) and (6.5), it turns into $K(x)K'(x)(1+x)/2$, and we obtain

$$\int_0^1 \frac{K(x)K'(x)}{1+x} dx = \frac{A}{2} + \frac{\pi^3}{32}. \quad (7.3)$$

It also follows that

$$\int_0^1 \frac{K(x)E'(x)}{1+x} dx = \frac{\pi}{4} \log 2 + \frac{\pi^3}{32}. \quad (7.4)$$

Letting $x \mapsto (1-x)/(1+x)$ in $K(x)K'(x)/(1+x)^2$, followed by quadratic transforms, gives

$$\int_0^1 \frac{K(x)K'(x)}{(1+x)^2} dx = \frac{A+B}{4} + \frac{\pi^3}{32}. \quad (7.5)$$

We integrate $x(1-x)/(1+x) K(x)K'(x)$ by parts; the evaluations (7.1) – (7.5), together with Legendre's relation, give

$$\int_0^1 \frac{E(x)K'(x)}{(1+x)^2} dx = \frac{A-B}{4} + \frac{\pi}{8} + \frac{\pi^3}{32}, \quad (7.6)$$

$$\int_0^1 \frac{K(x)E'(x)}{(1+x)^2} dx = \frac{B}{2} + \frac{\pi}{8}. \quad (7.7)$$

Armed with these two equations and integrating $x(1-x)/(1+x) K(x)E'(x)$ by parts, we have

$$\int_0^1 \frac{E(x)E'(x)}{(1+x)^2} dx = \frac{A-5B}{4} + \frac{\pi}{8} + \frac{\pi^3}{32}. \quad (7.8)$$

The desired evaluations have now all been found. \diamond

In fact, the quadratic transforms lead to

$$\int_0^1 \frac{K(x)K'(x)}{(1+x)^n} dx = \int_0^1 \left(\frac{1+x}{2} \right)^n K(x)K'(x), \quad (7.9)$$

where for positive integer n , the right hand side is a linear combination of A, B and π^3 , using the recursion satisfied by the moments of KK' (see Chapter 6, Section 6).

Thus (7.9) gives us the definite integrals of $KK'/(1+x)^n$ for all $n \in \mathbb{Z}$. Integrating $x(1-x)/(1+x)^{n-1}KK'$ and $x(1-x)/(1+x)^{n-1}KE'$ by parts, together with Legendre's relation, we obtain three equations relating the integral of $KE'/(1+x)^n, EK'/(1+x)^n, EE'/(1+x)^n$ to the same objects except with the

indices $n - 1$ and $n - 2$ (together with integrals involving KK' which we know from (7.9)). These three equations can be solved, see below. With the *starting values* (7.1) – (7.8), we thus obtain all the integrals of the form $F/(1+x)^n$ for integer $n > 0$, where F is one of KK', KE', EK', EE' . We observe that such integrals are always a rational linear combination of $A, B, \pi, \pi \log 2, \pi^3$. By running the recursions ‘backwards’, we note that the integrals of $F(x)(1+x)^n$ are also linear combinations of A, B, π, π^3 for integer $n \geq 0$. Thus we have the following:

Theorem 7.1. *For $n \in \mathbb{Z}$, let F be one of KK', KE', EK' or EE' , then*

$$\int_0^1 F(x)(1+x)^n dx$$

can be expressed as a \mathbb{Q} -linear combination of elements from the set $\{A, B, \pi, \pi \log 2, \pi^3\}$, where $\pi \log 2$ may appear only when $n = -1$, and where

$$A = \frac{\pi^3}{8} {}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1, 1 \end{matrix} \middle| 1\right), \quad B = \frac{\pi^3}{32} {}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{3}{2} \\ 1, 2, 2 \end{matrix} \middle| 1\right).$$

PROOF. The values of A and B are given in Chapter 6, Section 4. The constant $\pi \log 2$ essentially comes from Legendre’s relation, so by some inspection it does not occur when $n \neq -1$. By the discussion preceding the theorem, we only require the recursions below, and the starting values (7.1) – (7.8) given in Example 7.1.1.

We exhibit the recursions here: let KK'_n denote $\int_0^1 K(x)K'(x)/(1+x)^n dx$ (from (7.9), they can all be computed from the moments of KK'). The other integrals are denoted similarly, and in terms of KK'_n they are:

$$\begin{aligned} KE'_n &= \frac{\pi}{4(1+x)^n} + nKK'_n - \frac{3n-2}{2}KK'_{n-1} + \frac{n-1}{2}KK'_{n-2}, \\ EK'_n &= \frac{\pi}{4(1+x)^n} - (n-1)KK'_n + \frac{3n-2}{2}KK'_{n-1} - \frac{n-1}{2}KK'_{n-2}, \\ EE'_n &= \frac{\pi x(x(3-n) + n)}{4(1+x)^n} - (1-n)(1-2n)KK'_n + \frac{12n^2 - 31n + 22}{2}KK'_{n-1} \\ &\quad - \frac{13n^2 - 48n + 47}{2}KK'_{n-2} + \frac{6n^2 - 29n + 36}{2}KK'_{n-3} - \frac{(n-3)^2}{2}KK'_{n-4}. \end{aligned}$$

□

Remark 7.1.1. We know that

$$\int_0^1 \frac{E(x)}{1+x} dx = 1, \quad \int_0^1 \frac{K(x)}{1+x} dx = \frac{\pi^2}{8}.$$

Using integration by parts, we have

$$\int_0^1 \frac{nE(x)}{(1+x)^{n+1}} dx = \frac{1}{2^n} + \int_0^1 \frac{K(x)}{(1+x)^n} + \frac{(n-2)E(x)}{(1+x)^n} dx,$$

$$\int_0^1 \frac{2nK(x)}{(1+x)^{n+1}} dx = \int_0^1 \frac{(3n-1)K(x)}{(1+x)^n} - \frac{(n-1)K(x)}{(1+x)^{n-1}} - \frac{E(x)}{(1+x)^{n+1}} dx.$$

Therefore, for integer n , all integrals of the form $\int_0^1 E(x)(1+x)^n dx$, $\int_0^1 K(x)(1+x)^n dx$ can be expressed as a \mathbb{Q} -linear combination of elements from $\{1, \pi^2\}$.

A very similar argument, using the starting values

$$\int_0^1 \frac{E'(x)}{1+x} dx = 2G - 1, \quad \int_0^1 \frac{K'(x)}{1+x} dx = 2G,$$

shows that for all integer n , integrals of the form $\int_0^1 E'(x)(1+x)^n dx$, $\int_0^1 K'(x)(1+x)^n dx$ can be expressed as a \mathbb{Q} -linear combination of elements of $\{1, G\}$. Here, as usual, G denotes Catalan's constant. \diamond

7.2. Two complementary elliptic integrals

In this section we further analyse integrals which contain the product of two complementary elliptic integrals. Let C denote $\int_0^1 K'(x)^2 dx$ and let D denote $\int_0^1 x^2 K'(x)^2 dx$. From Chapter 6 it is known that $\int_0^1 E(x)K(x)/(1+x) dx = C/4$, and some manipulations involving quadratic transforms lead to

$$\int_0^1 \frac{E'(x)K'(x)}{1+x} dx = \frac{7\zeta(3)}{4}. \quad (7.10)$$

As was done in Example 7.1.1, our first aim is to produce integrals of the above form with denominators $(1+x)$ and $(1+x)^2$, and then find recursions when $(1+x)^n$ is involved. Indeed, integration by parts using $x(1-x)E'(x)^2$, $x(1-x)K'(x)^2$ and $x(1-x)E'(x)K(x)$ gives

$$\int_0^1 \frac{K'(x)^2}{1+x} dx = \frac{7\zeta(3)}{4} + \frac{C}{2}, \quad (7.11)$$

$$\int_0^1 \frac{E'(x)^2}{1+x} dx = \frac{7\zeta(3)}{4} - \frac{1}{2} - \frac{D}{2}. \quad (7.12)$$

Similarly, integrating the same functions divided by $(1+x)$ by parts, we obtain

$$\int_0^1 \frac{E'(x)K'(x)}{(1+x)^2} dx = 1 + \frac{D}{2}, \quad (7.13)$$

$$\int_0^1 \frac{K'(x)^2}{(1+x)^2} dx = \frac{1}{2} + \frac{7\zeta(3)}{4} + \frac{C+D}{4}, \quad (7.14)$$

$$\int_0^1 \frac{E'(x)^2}{(1+x)^2} dx = \frac{5}{2} - \frac{7\zeta(3)}{4} + \frac{7D-C}{4}. \quad (7.15)$$

Finally, integrating the aforementioned functions divided by $(1+x)^n$ by parts, we produce second order recursions in terms of n . The recursions, like those in the proof of Theorem 7.1, are rather involved and we do not exhibit them here. We can also run the recursion backwards to account for negative integer n 's (so for instance $\int_0^1 (1+x)^2 E'(x)K'(x) dx = 1/2 + 7\zeta(3)/4 + (5C - D)/9$). In summary, we have actually a proof of the following:

Theorem 7.2. *For $n \in \mathbb{Z}$, let F be one of E'^2 , EK' or K'^2 , then*

$$\int_0^1 F(x)(1+x)^n dx$$

can be expressed as a \mathbb{Q} -linear combination of elements from the set $\{1, \zeta(3), C, D\}$, where

$$C = \int_0^1 K'(x)^2 dx, \quad D = \int_0^1 x^2 K'(x)^2 dx,$$

and their ${}_{7F_6}$ representations are given in Chapter 6, Section 3.

Remark 7.2.1. Evaluations in this section in terms of $\zeta(3)$, such as (7.10), were first discovered experimentally using PSLQ. Those discoveries convinced the author of the existence of transformations from the integrals involved to odd moments of $F(x)$, and proofs were soon found. \diamond

7.3. Two elliptic integrals

We established in Theorem 6.4 that

$$\int_0^1 \frac{E(x)K(x)}{1+x} dx = \frac{C}{4}.$$

Similarly,

$$\int_0^1 \frac{K(x)^2}{1+x} dx = \frac{7\zeta(3)}{16} + \frac{C}{4}.$$

A quadratic transform gives

$$\int_0^1 \frac{2K'(x)^2}{(1+x)^2} dx = \int_0^1 (1+x)^2 K(x)^2 dx,$$

and since the left hand side is known from the last section, we deduce that

$$\int_0^1 x^2 K(x)^2 dx = 1 + \frac{D}{2}. \quad (7.16)$$

As noted in Chapter 6, among moments of products of two elliptic integrals, there were only five that we did not possess closed forms of:

$$E(x)^2, x^2 E(x)^2, E(x)K(x), x^2 E(x)K(x), x^2 K(x)^2,$$

since only four independent linear relations connecting them were found. Importantly, equation (7.16) is the desired fifth independent relation. Thus, studying integrals of $F(x)(1+x)^n$ (in particular, $K'(x)^2/(1+x)^2$) brings about the resolution of the Conjecture 6.1. We now have:

$$\int_0^1 E(x)^2 dx = \frac{4+C+D}{6}, \quad (7.17)$$

$$\int_0^1 x^2 E(x)^2 dx = \frac{44-C+11D}{90}, \quad (7.18)$$

$$\int_0^1 E(x)K(x) dx = \frac{2+C+D}{4}, \quad (7.19)$$

$$\int_0^1 x^2 E(x)K(x) dx = \frac{26-C+11D}{36}. \quad (7.20)$$

Proposition 7.1. *Conjecture 6.1 is true.*

PROOF. Using the closed forms found above, the conjecture reduces to the equivalent form

$$\int_0^1 2E'(x)K'(x) dx = C - D,$$

which has been proved in Chapter 6, equation (6.57). \square

Continuing, we find with integration by parts, armed with our new closed forms:

$$\begin{aligned} \int_0^1 \frac{E(x)^2}{1+x} dx &= \frac{C-D}{4}, & \int_0^1 \frac{E(x)^2}{(1+x)^2} dx &= \frac{1+D}{2}, \\ \int_0^1 \frac{K(x)^2}{(1+x)^2} dx &= \frac{7\zeta(3)}{16} + \frac{C+D}{8}, & \int_0^1 \frac{E(x)K(x)}{(1+x)^2} dx &= \frac{7\zeta(3)}{16} + \frac{C-D}{8}. \end{aligned}$$

Thus all the starting values are given; as was done in the last two sections, recursions based on these values can be found; again we omit the unpleasant details. In summary, we have

Theorem 7.3. For $n \in \mathbb{Z}$, let F be one of E^2 , EK or K^2 , then

$$\int_0^1 F(x)(1+x)^n dx$$

can be expressed as a \mathbb{Q} -linear combination of elements from the set $\{1, \zeta(3), C, D\}$, and where

$$C = \int_0^1 K'(x)^2 dx, \quad D = \int_0^1 x^2 K'(x)^2 dx.$$

From the results in these three sections, we have succeeded in proving

Corollary 7.1. For $n \in \mathbb{Z}$ and G a product of up to two elliptic integrals, $\int_0^1 G(x)(1+x)^n dx$ can be written as a \mathbb{Q} -linear combination of elements taken from a small set S of special constants, where

$$S = \{1, \pi, \pi^2, \pi^3, \pi \log 2, G, \zeta(3), A, B, C, D\}.$$

7.4. More on explicit primitives

A small number of functions with explicit primitives are listed in Section 6, Chapter 6. We now return to this topic more systematically and add a few more results.

First we claim that for *odd* $n > 0$, we may find explicit primitives of $x^n K(x)$ and $x^n E(x)$. Indeed, the claim is easy for $n = 1$. Now, integrating $x^{n+2} K(x)$ by parts, we obtain

$$\int x^{n+2} K(x) dx = \frac{x^{n+1}}{n+2} (E(x) + (x^2 - 1)K(x)) + \frac{n+1}{n+2} \int x^n (K(x) - E(x)) dx.$$

This allows us to find the primitive of $x^{n+2} K(x)$. For $x^{n+2} E(x)$, simply observe that

$$\int x^{n+2} ((n+4)E(x) - K(x)) dx = x^{n+3} E(x).$$

Therefore, the claim is proven inductively.

Next, for *even* $n < 0$, we may find explicit primitives of $x^n K(x)$ and $x^n E(x)$. Again, the base case is simple. The inductive step follows easily from the pair of equations:

$$\int \frac{(2-n)E(x) - K(x)}{x^n} dx = \frac{E(x)}{x^{n-1}},$$

$$\int \frac{E(x) + ((n-2)x^2 - n)K(x)}{x^n} dx = \frac{(1-x^2)K(x)}{x^{n-1}}.$$

Now, for *odd* $n > 0$, and for *even* $n < 0$, explicit primitives of $x^n K'(x)$ and $x^n E'(x)$ can be found. The relevant equations are

$$\int x^n (E'(x) + ((n+2)x^2 - (n+1))K'(x)) dx = x^{n+1}(x^2 - 1)K'(x),$$

$$\int x^n (((4+n)x^2 - (n+1))E'(x) - x^2 K'(x)) dx = x^{n+1}(x^2 - 1)E'(x).$$

Therefore, by letting $x \mapsto x'$, and using F to denote one of the four elliptic integrals, we see that there exists an explicit primitive for $\frac{x F(x)}{x'^m}$, where $m > 1$ is *odd* – this generalises a result in [101] and a number of results scattered around integral tables elsewhere.

By a quadratic transform, we also obtain the closed forms for the integrals of $(1-x)^n/(1+x)^{n+1} K(x)$ or $K'(x)$, for $n > 0$ *odd* or $n < 0$ *even*.

Moreover, since $\int E(x)/(1 \pm x) dx$ has a closed form, using partial fractions and the results above, we can obtain the explicit integral for $x^n E(x)/(1-x^2)$, with $n > 0$ *odd*, $n < 0$ *even*, or $n = 0$. By $x \mapsto x'$, this gives the primitive for $E'(x)/(x x'^m)$, with $m > 0$ *odd* or $m = 0$.

Finally, we record the primitives $\int x^n ((n+1)K'(x) - (n+2)E'(x)) dx = x^{n+1}(K'(x) - E'(x))$ and $\int x^n ((n+2)E(x) - K(x)) dx = x^{n+1}E(x)$; a few more are found in [104, section 5.1].

7.5. Some other integrals

7.5.1. Better expression of the moments. By applying Thomae's ${}_3F_2$ transform [25, p. 14], we see that the n th moment of K can be nicely expressed as

$$\int_0^1 x^n K(x) dx = {}_3F_2\left(1, 1, \frac{1-n}{2} \mid \frac{3}{2}, \frac{3}{2} \mid 1\right), \quad (7.21)$$

and this form often allows us to interchange the order of summation when the left hand integral appears in a sum.

For instance, interchanging the order of summation allows us to obtain

$$\int_0^1 \frac{x}{1-tx^2} K(x) dx = \frac{1}{1-t} {}_3F_2\left(1, 1, 1 \mid \frac{3}{2}, \frac{3}{2} \mid \frac{t}{t-1}\right). \quad (7.22)$$

Similarly, the n th moment of E is

$$\frac{2}{3} {}_3F_2\left(1, 2, \frac{1-n}{2} \mid \frac{3}{2}, \frac{5}{2} \mid 1\right),$$

so the generating function for the odd moments is

$$\int_0^1 \frac{x}{1-tx^2} E(x) dx = \frac{2}{3(1-t)} {}_3F_2\left(\begin{matrix} 1, 1, 2 \\ \frac{3}{2}, \frac{5}{2} \end{matrix} \middle| \frac{t}{t-1}\right).$$

As a harder example, consider the integral $\int_0^1 xK(x/\sqrt{2})K(x) dx$. Expand $xK(x/\sqrt{2})$ as a series, interchange the order of summation and integration, apply (7.21) and finally interchange the order of summation. The resulting inner sum is a ${}_2F_1$ with argument $1/2$ which simplifies [25, p. 11]. Therefore we obtain

$$\int_0^1 \frac{\sqrt{\pi}x}{2} K\left(\frac{x}{\sqrt{2}}\right) K(x) dx = \frac{\Gamma^2(\frac{1}{4})}{8} {}_5F_4\left(\begin{matrix} \frac{1}{4}, \frac{1}{4}, \frac{1}{2}, 1, 1 \\ \frac{3}{4}, \frac{3}{4}, \frac{5}{4}, \frac{5}{4} \end{matrix} \middle| 1\right) + \frac{\Gamma^2(\frac{3}{4})}{9} {}_5F_4\left(\begin{matrix} \frac{3}{4}, \frac{3}{4}, 1, 1, \frac{3}{2} \\ \frac{5}{4}, \frac{5}{4}, \frac{7}{4}, \frac{7}{4} \end{matrix} \middle| 1\right).$$

7.5.2. Differentiation. We may differentiate the results in Theorem 6.3 with respect to t , and produce integrals such as

$$\begin{aligned} \int_0^1 \frac{K'(x)}{(1+x^2)^2} dx &= \sqrt{\frac{\pi}{2}} \left[\frac{\pi^2}{4\Gamma^2(\frac{1}{4})} + \frac{3\Gamma^2(\frac{1}{4})}{32} \right], \\ \int_0^1 \frac{xK(x)K'(x)}{(1+x^2)^2} dx &= \frac{\pi^2}{32} + \Gamma^4\left(\frac{5}{4}\right). \end{aligned} \quad (7.23)$$

By a quadratic transform, we have

$$\int_0^1 \frac{xK(x)K'(x)}{1+x^2} dx = \int_0^1 \frac{K(x)K'(x)}{1+x^2} dx - \frac{1}{2} \int_0^1 K(x)K'(x) dx, \quad (7.24)$$

thus the middle term may be expressed in closed form using (6.30). So, by partial fractions, the moments

$$\int_0^1 \frac{x^n}{1+x^2} K(x)K'(x) dx$$

can all be worked out for positive integers n .

7.5.3. Logarithms. A number of integrals involving E , K and logs can be computed using integration by parts (and many are already known [66]). For example,

$$\int x \log(x) K(x) dx = (\log(x) - 2)E(x) + (1 - \log(x))(1 - x^2)K(x).$$

Many such integrals are possible, e. g. if we replaced K by E or used a higher power of x . We give one more example:

$$\int \frac{\log(1-x)}{x} (E(x) - K(x)) dx = (1+x)K(x) + (\log(1-x) - 1)E(x).$$

Remark 7.5.1. On the other hand, the constant $\log 2$ appears in some definite integrals (see also Theorem 7.1). Using the series for $E(x)$, we have

$$\int_0^1 \frac{E(x) - \pi/2}{x} dx = -\frac{\pi}{16} {}_4F_3\left(\begin{matrix} \frac{1}{2}, 1, 1, \frac{3}{2} \\ 2, 2, 2 \end{matrix} \middle| 1\right) = 1 - 2G - \frac{\pi}{2} + \pi \log 2,$$

where the last equality follows from a contiguous relation and a ${}_4F_3$ identity [3, Prop. 2.1]. Similarly,

$$\int_0^1 \frac{K(x) - \pi/2}{x} dx = \pi \log 2 - 2G;$$

compare with (6.31). ◇

7.5.4. More results on two elliptic integrals. We collect some miscellaneous integrals involving the product of two elliptic integrals.

Example 7.5.1. Whilst we may easily add and subtract the moments of $K'K$, $K'E$ etc. obtained in Chapter 6 Section 4, a few extra relations may be obtained by using the ${}_2F_1$ representation of $K - E$ (6.64) due to its double zero at the origin, namely:

$$\begin{aligned} \int_0^1 \frac{K'(x)}{x} (K(x) - E(x)) dx &= \frac{\pi \log 2}{2}, & \int_0^1 \frac{E'(x)}{x} (K(x) - E(x)) dx &= \frac{\pi}{4}, \\ \int_0^1 \frac{K'(x)}{x^2} (K(x) - E(x)) dx &= \int_0^1 K(x) E'(x) dx, \\ \int_0^1 \frac{E'(x)}{x^2} (K(x) - E(x)) dx &= \int_0^1 K'(x) E(x) - K(x) E'(x) dx. \end{aligned}$$

◇

Example 7.5.2. By using quadratic transforms, $x \mapsto x'$, and integration by parts, we have the following chain of equalities:

$$\begin{aligned} \int_0^1 \frac{K'(x)^2}{x'} dx &= \int_0^1 \frac{K(x)^2}{x'} dx = 2 \int_0^1 \frac{E(x)K(x)}{x'} dx \\ &= \int_0^1 \frac{1+x}{\sqrt{x}} K(x)^2 dx = \int_0^1 \frac{1+x}{4\sqrt{x}} K'(x)^2 dx. \end{aligned} \tag{7.25}$$

The last term is a linear combination of moments of K'^2 , and so (7.25) may be written as the sum of two ${}_7F_6$'s (Chapter 6, Section 3). Since quadratic transform also gives

$$\int_0^1 K(x)^2 dx = \int_0^1 \frac{1-x}{\sqrt{x}} K(x)^2 dx,$$

we may combine the last formula with (7.25) to produce closed forms for the integrals of $K(x)^2/\sqrt{x}$ and $K(x)^2\sqrt{x}$. Other fractional moments of K^2 seem beyond our reach. \diamond

7.6. Incomplete moments

We may use a special case of the Clausen's formula [11, p. 116]

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| t\right) = \frac{4}{\pi^2} K\left(\sqrt{\frac{1-\sqrt{1-t}}{2}}\right)^2 \quad (7.26)$$

to produce some incomplete moments.

As an example, multiply both sides of (7.26) by t^n , integrate from $t = 0$ to 1 followed by a change of variable. We obtain

$$\int_0^{1/\sqrt{2}} x^{2n+1}(1-x^2)^n(1-2x^2)K(x)^2 dx = \frac{\pi^2}{2^{2n+5}(n+1)} {}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, n+1 \\ 1, 1, n+2 \end{matrix} \middle| 1\right).$$

In fact, the integral with respect to t of (7.26) is $t {}_3F_2(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 2; t)$, which has a closed form because it is contiguous to the ${}_3F_2$ in (7.26) (see Chapter 14). The closed form is, using $X = \sqrt{\frac{1-\sqrt{1-t}}{2}}$,

$$\int K(X)^2 dt = 4(1 + \sqrt{1-t})E(X)K(X) - 4E(X)^2 - 2(1 + \sqrt{1-t} - t)K(X)^2.$$

Therefore, a number of incomplete moments where the limits of integration are singular values may be expressed in closed form; for instance,

$$\begin{aligned} \int_0^{1/\sqrt{2}} x(1-2x^2)K(x)^2 dx &= \frac{\Gamma^4(\frac{1}{4})}{128\pi} - \frac{\pi^3}{2\Gamma^4(\frac{1}{4})}, \\ \int_0^{3-2\sqrt{2}} x(1-2x^2)K(x)^2 dx &= \frac{(\sqrt{2}-1)^3\pi}{4} \left[1 - \frac{4\pi^2}{(\sqrt{2}-1)\Gamma^4(\frac{1}{4})} + \frac{(\sqrt{2}-1)^2\Gamma^4(\frac{1}{4})}{16\pi^2} \right]. \end{aligned} \quad (7.27)$$

For the integrand below, we can use (7.26) to write it as a ${}_3F_2$ series. Interchanging the order of summation and integration, and using the evaluation of a ${}_2F_1$ at $1/2$ [25], we have

$$\begin{aligned} \int_0^{1/\sqrt{2}} K(x)^2 x^{2a}(x')^{2a-1} dx &= \int_{1/\sqrt{2}}^1 K'(x)^2 x^{2a}(x')^{2a-1} dx \\ &= \frac{\pi^{\frac{5}{2}} \Gamma(\frac{1}{2} + a)}{4^{a+2} \Gamma(1 + a)} {}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} + a \\ 1, 1, 1 + a \end{matrix} \middle| 1\right). \end{aligned} \quad (7.28)$$

We can therefore work out all these odd incomplete moments of K^2 . A special case is

$$\int_0^{1/\sqrt{2}} xK(x)^2 dx = \int_{1/\sqrt{2}}^1 xK'(x)^2 dx = \frac{\pi G}{4}.$$

A similar analysis can be done with a range of ${}_3F_2$'s, for instance, using contiguous relations in Chapter 14,

$$\frac{\pi^2}{4} {}_3F_2\left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| 4x^2(1-x^2)\right) = K(x)^2 - 2E(x)K(x) + 2E(x)^2.$$

When combined with (7.28), we get for instance

$$\int_0^{1/\sqrt{2}} xE(x)(K(x) - E(x)) dx = \frac{\pi}{32}(2G - 1).$$

We can also apply quadratic transforms on (7.28), an example being

$$\int_0^{3-2\sqrt{2}} \frac{1-x}{1+x} K(x)^2 dx = \frac{\pi G}{8}.$$

Finally, by using the derivative of a ${}_5F_4$ recorded in [111], other kinds of results may be obtained, such as

$$\int_0^{1/\sqrt{2}} \frac{1-2x^2}{x(1-x^2)} (4K(x)^2 - \pi^2) dx = \frac{\pi^2}{16} {}_5F_4\left(\begin{matrix} 1, 1, \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \\ 2, 2, 2, 2 \end{matrix} \middle| 1\right).$$

7.7. One elliptic integral with parameters

In this section we prove a number of integrals involving a single elliptic integral and several parameters.

Example 7.7.1. We first use a transform relating $K^{1/4}$ to K (in the notation of Chapter 5),

$${}_2F_1\left(\begin{matrix} \frac{1}{4}, \frac{3}{4} \\ 1 \end{matrix} \middle| t^2\right) = \frac{1}{\sqrt{1+t}} {}_2F_1\left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| \frac{2t}{1+t}\right), \quad (7.29)$$

then evaluate the general moments of the left hand side, which translate to

$$J(a, b) := \int_0^1 \frac{x^{2a} x^{b/2} K(x)}{(2-x^2)^{a+b+1}} dx = \frac{\pi \Gamma(\frac{2a+1}{4}) \Gamma(\frac{b+2}{2})}{2^{b+\frac{7}{2}} \Gamma(\frac{2a+2b+5}{4})} {}_3F_2\left(\begin{matrix} \frac{1}{4}, \frac{3}{4}, \frac{2a+1}{4} \\ 1, \frac{2a+2b+5}{4} \end{matrix} \middle| 1\right). \quad (7.30)$$

This generalises an entry in [101]. Now via quadratic transforms, we also get

$$J(a, b) = \int_0^1 \frac{x^{a-1/2}(1-x^2)^{b+1}}{2^{b-a+1}(1+x^2)^{a+b+1}} K(x) dx = \int_0^1 \frac{2^b x^{b/2} (1-x)^{2a} (1+x)^{b+1}}{(1+6x+x^2)^{a+b+1}} K'(x) dx. \quad (7.31)$$

Letting $x \mapsto x'$ in any of the integrals for $J(a, b)$ also gives reformulations. In some cases, we can evaluate the right hand side of $J(a, b)$ using Dixon's theorem or Clausen's formula. A special case of the second equality in (7.31) is

$$\int_0^1 \frac{(1-x)^{2a}}{(1+x)^a x^{\frac{a+1}{2}}} K'(x) dx = \frac{\pi}{2^{\frac{3}{2}-2a}} \frac{\Gamma^2(\frac{1-a}{2})\Gamma(\frac{1+2a}{4})}{\Gamma^2(\frac{3}{4})\Gamma(\frac{3-2a}{4})}.$$

Other examples include

$$\sqrt{2} \int_0^1 \frac{K(x)}{\sqrt{1+x^2}} dx = \int_0^1 \frac{K'(x)}{\sqrt{1+x^2}} dx = \frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{32\sqrt{2}\pi}, \quad (7.32)$$

where the first equality is also a special case of (7.36) (after $x \mapsto x'$, with $b = -c = 1/2$). \diamond

Example 7.7.2. Using the transform [46, Prop. 5.6]

$$K(t) = \frac{\pi}{2} {}_2F_1\left(\frac{1}{4}, \frac{1}{4} \middle| 4t^2(1-t^2)\right),$$

we replace K below by the ${}_2F_1$ and make a change of variable. The result is (as recorded in [101])

$$\int_0^1 K\left(\frac{x}{\sqrt{2}}\right) x^{2a+1} (1-x^2)^{b-1} (2-x^2)^b dx = \frac{\pi}{8} \frac{\Gamma(a+1)\Gamma(\frac{b}{2})}{\Gamma(a+\frac{b}{2}+1)} {}_3F_2\left(\frac{1}{4}, \frac{1}{4}, a+1 \middle| 1, a+\frac{b}{2}+1\right). \quad (7.33)$$

The right hand side sometimes simplifies, e. g.

$$\int_0^1 \frac{K\left(\frac{x}{\sqrt{2}}\right)}{\sqrt{(1-x^2)(2-x^2)}} dx = \frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{32\sqrt{2}\pi}.$$

\diamond

Example 7.7.3. By using a quadratic transform followed by a change of variables, we have

$$\int_0^1 K'(x)(1+x)^a(1-x)^b x^c dx = 2^{a+b+1} \int_0^1 \frac{x^b(1-x)^c}{(1+x)^{a+b+c+1}} K(x) dx. \quad (7.34)$$

In some cases, the left hand side can be evaluated in closed form by writing the rational function as a series and interchanging the order of integration and summation. On the other hand, we may sometimes integrate the right hand side term by term after expanding K as a series. A similar relation holds for E :

$$\int_0^1 (1+x)^a(1-x)^b x^c (E'(x) + xK'(x)) dx = 2^{a+b+2} \int_0^1 \frac{x^b(1-x)^c}{(1+x)^{a+b+c+3}} E(x) dx.$$

Some consequences of the development above include

$$\int_0^1 \frac{K'(x)}{\sqrt{1+x}} dx = \sqrt{2} \int_0^1 \frac{K(x)}{\sqrt{1+x}} dx, \quad (7.35)$$

$$\int_0^1 \frac{K'(x)}{\sqrt{x(1+x)}} dx = \int_0^1 \frac{\sqrt{2}K(x)}{\sqrt{1-x}} dx = \int_0^1 \frac{K'(x)}{\sqrt{2x(1-x)}} dx = \int_0^1 \frac{K(x)}{\sqrt{x(1-x)}} dx.$$

The second line evaluates to $\frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{16\pi}$ by Whipple's formula for a ${}_3F_2$ at 1 [25]; note that this constant (and its algebraic multiples) appears often in this section.

We will return to the evaluation of the first line (7.35) later. \diamond

Example 7.7.4. Also recorded in [101] is the identity

$$\int_0^1 x(1-x^2)^{b-1}(1-zx^2)^c K(x) dx = \frac{\pi(1-z)^c \Gamma^2(b)}{4\Gamma^2(b+\frac{1}{2})} {}_3F_2 \left(\begin{matrix} b, b, -c \\ b+\frac{1}{2}, b+\frac{1}{2} \end{matrix} \middle| \frac{z}{z-1} \right). \quad (7.36)$$

(A similar formula holds when K is replaced by E .) An equivalent form is

$$\int_0^1 x^{2b-1}(1-zx^2)^c K'(x) dx = \frac{\pi \Gamma^2(b)}{4\Gamma^2(b+\frac{1}{2})} {}_3F_2 \left(\begin{matrix} b, b, -c \\ b+\frac{1}{2}, b+\frac{1}{2} \end{matrix} \middle| z \right).$$

The proof is illustrative:

PROOF OF (7.36). We expand $K(x)$ as a series and interchange the order of integration and summation. The integral is of Euler type (4.3) and produces ${}_2F_1(-c, 1+k; 1+k+b; z)$. We then apply one of Euler's transforms (6.32), sending the ${}_2F_1$ to

$$(1-z)^c {}_2F_1 \left(\begin{matrix} -c, -b \\ 1+k-b \end{matrix} \middle| \frac{z}{z-1} \right).$$

Importantly, this *reduces* the dependence of the ${}_2F_1$ parameters on k . Having done so, we write the ${}_2F_1$ as a sum and interchange the order of summation. The inner k sum is now simpler, being a ${}_2F_1$ with argument 1. The right hand side of (7.36) follows by completing the outer summation. \square

7.8. Fourier series and three elliptic integrals

It is remarked below Theorem 6.5 that based on numerical evidence, the integrals of K'^3 and K^2K' are related by a rational multiple, namely

$$\int_0^1 K'(x)^3 dx = 3 \int_0^1 K(x)^2 K'(x) dx. \quad (7.37)$$

We prove this observation here.

Lemma 7.1. *For any function F where the integrals below converge and where the sum and integral may be interchanged,*

$$\sum_{n=0}^{\infty} \int_0^{\pi/2} \frac{\Gamma^2(n + \frac{1}{2})}{\Gamma^2(n + 1)} \cos((4n+2)t) \cos(t) F(\sin t) dt = \int_0^1 (x'K'(x) - xK(x)) F(x) dx. \quad (7.38)$$

PROOF. We write the right hand side as a Fourier series (6.39); the trigonometric coefficients are

$$\cos(t) \cos((4n + 1)t) - \sin(t) \sin((4n + 1)t) = \cos((4n + 2)t),$$

which correspond to the coefficients on the left hand side. \square

Remark 7.8.1. Clearly, if the right hand side of (7.38) used $+$ instead of $-$, then the left hand side would have $\cos(4nt)$ instead of $\cos((4n + 2)t)$. If the right hand side had $xK' \pm x'K$, then $\sin((4n + 1 \pm 1)t)$ would appear on the left. Similar trigonometric manipulations also lead to identities such as

$$\int_0^1 (K(x) + K'(x)) F(x) \frac{dx}{\sqrt{2}} = \sum_{n=0}^{\infty} \int_0^{\pi/2} \frac{\Gamma^2(n + \frac{1}{2})}{\Gamma^2(n + 1)} \sin\left((4n+1)t + \frac{\pi}{4}\right) \cos(t) F(\sin t) dt,$$

and

$$2K(e^{2ix}) = e^{-ix} (K(\cos x) + iK(\sin x)). \quad (7.39)$$

An equivalent expression for the left hand side of (7.38) is

$$\sum_{n=0}^{\infty} \int_0^1 \frac{\Gamma^2(n + \frac{1}{2})}{\Gamma^2(n + 1)} T_{4n+2}(x) F(x) dx,$$

where $T_n(x) = \cos(n \cos^{-1} x)$ denotes the *Chebyshev polynomial of the first kind*. Indeed, when $n = 0$, this leads to

$$\int_0^1 \frac{2x^2 - 1}{x'} K(x)^2 dx = \frac{\pi^3}{8}, \quad (7.40)$$

an identity first observed *experimentally*, and it is in the attempt to prove (7.40) that the Lemma 7.1 was discovered. A more general form of (7.40) is

$$\int_0^1 \frac{T_{2n}(x)}{x'} K(x)^2 dx = \frac{\pi^2 \Gamma^2(\frac{n+1}{2})}{4 \Gamma^2(\frac{n+2}{2})} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{n+1}{2}, \frac{n+1}{2} \\ 1, \frac{n+2}{2}, \frac{n+2}{2} \end{matrix} \middle| 1 \right).$$

\diamond

We continue our proof of (7.37). In (7.38), take $F(x) = K(x)^2/x'$. The right hand side can be simplified by $x \mapsto x'$, and on the left hand side, orthogonality causes massive cancellations to occur. The result is

$$\sum_{n=0}^{\infty} \frac{\pi^2 \Gamma^4(n + \frac{1}{2})}{8 \Gamma^4(n + 1)} {}_4F_3 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, -n, -n \\ 1, \frac{1}{2} - n, \frac{1}{2} - n \end{matrix} \middle| 1 \right) = \int_0^1 K'(x)^3 - K(x)^2 K'(x) dx. \quad (7.41)$$

However, the left hand side is precisely $2 \int_0^1 K(x)^2 K'(x) dx$, as established in (6.68). The key result (7.37) then follows, linking together the two groups of integrals mentioned in Theorem 6.5. An evaluation of (7.37) in terms of Gamma functions is described in the next section.

Remark 7.8.2. The quadratic transforms for K may be written in terms of trigonometric variables:

$$\cos^2 t K(\sin 2t) = K(\tan^2 t). \quad (7.42)$$

The change of variable $x \mapsto \tan^2 t$, followed by applying (7.42) and expansion into the Fourier series can be quite effective. \diamond

7.9. Proof of the conjecture

It is expected that closed form evaluations of the integral of the cube of a special function are rare. Therefore a large portion of the recent work [169] is devoted to two such evaluations, including a proof of an equivalent form of Conjecture 6.2,

$$\int_0^1 x K'(x)^3 dx = \frac{\Gamma^8(\frac{1}{4})}{640\pi^2}. \quad (7.43)$$

We summarise the main argument in [169] and some other results here.

We start with the parametrisations in terms of Jacobi's *theta functions* [46, Ch. 2], with $\log q = -\pi K'(k)/K(k)$,

$$K(k) = \frac{\pi}{2} \theta_3^2(q), \quad k = \frac{\theta_2^2(q)}{\theta_3^2(q)}, \quad k' = \frac{\theta_4^2(q)}{\theta_3^2(q)}, \quad \frac{dk}{dq} = \frac{\theta_2^2(q)\theta_4^4(q)}{2q\theta_3^2(q)}.$$

Therefore, we can write the integral in (7.43) (which we call I) as

$$I = \int_0^1 \frac{-\log^3 q}{16q} \theta_2^4(q)\theta_3^2(q)\theta_4^4(q) dq = \int_0^1 \frac{-\log^3 q}{q} \eta^4(q)\eta^2(q^2)\eta^4(q^4) dq, \quad (7.44)$$

where we have written the θ functions in terms of the Dedekind η function (3.40).

Now with $q = e^{2\pi i\tau}$, $f(\tau) = \eta^4(\tau)\eta^2(2\tau)\eta^4(4\tau)$ is a weight 5 *cusp form* (see e.g.

[12, 176]), and admits a Fourier series

$$f(\tau) = \sum_{n=1}^{\infty} a_n e^{2\pi i n \tau}. \quad (7.45)$$

Therefore the last integral in (7.44) is the following L -series (as can be seen by taking a Mellin transform):

$$I = 6 \sum_{n=1}^{\infty} \frac{a_n}{n^4}.$$

This is known as a *critical* L -value of f , $L(f, 4)$. It can be shown by standard methods [100] that in fact

$$f(\tau) = \frac{1}{4} \sum_{m, n=-\infty}^{\infty} (n - im)^4 q^{n^2 + m^2},$$

and so our integral reduces to

$$I = \frac{3}{2} \sum'_{m, n} \frac{(n - im)^4}{(n^2 + m^2)^4} = \frac{3}{2} \sum'_{m, n} \frac{1}{(n + im)^4}.$$

The prime means the $m = n = 0$ term is omitted in the sum. It is a known property of the Weierstrass invariant g_2 (an Eisenstein series) that

$$\frac{4}{15} g_2(\tau) = \sum'_{n, m} \frac{1}{(n + \tau m)^4} = \frac{16}{45} (1 - k^2 + k^4) K^4(k), \quad (7.46)$$

which, when evaluated at $\tau = i$ (corresponding to the first singular value), gives a closed form for I , and hence equation (7.43) follows.

We note that similar calculations give $L(f, 3) = \frac{1}{2\pi} \int_0^1 x K'(x)^2 K(x) dx$ ($L(f, 3)$ is the L -series with n^3 in the denominator). By (7.37) and Theorem 6.5, $L(f, 4) = 2\pi/5 L(f, 3)$. This way all critical L -values of f are related by π and rational constants.

Using $L(f, 3)$, the multiplicativity of the coefficients of f [143], and results from [205], we deduce the new lattice sums

$$\sum'_{m, n} \frac{(-1)^{m+n} m^2 n^2}{(m^2 + n^2)^3} = \frac{\Gamma^8(\frac{1}{4})}{2^9 3 \pi^3} - \frac{\pi \log 2}{8}, \quad (7.47)$$

$$\sum'_{m, n} \frac{(-1)^{m+n} m^4}{(m^2 + n^2)^3} = -\frac{\Gamma^8(\frac{1}{4})}{2^9 3 \pi^3} - \frac{3\pi \log 2}{8}, \quad (7.48)$$

$$\sum'_{m, n} \frac{(-1)^m m^2 n^2}{(m^2 + n^2)^3} = -\frac{\Gamma^8(\frac{1}{4})}{2^{10} 3 \pi^3} - \frac{\pi \log 2}{16}. \quad (7.49)$$

Remark 7.9.1. It can also be shown (W. Zudilin, private communication, Feb 2013), using techniques found in [212], that

$$L(g, 4) = \frac{\pi^2}{3} L\left(\frac{\eta^{12}(\tau)\eta^8(4\tau)}{\eta^{10}(2\tau)}, 2\right),$$

thus, writing the right hand side as an integral, we obtain

$$\begin{aligned} \frac{\Gamma^8(\frac{1}{4})}{1280\pi^2} &= \int_0^1 k^2 K(k) K'(k)^2 dk = \int_0^1 k k' K(k)^2 K'(k) dk \\ &= \int_0^1 \frac{(1-k)^2}{1+k} K(k)^2 K'(k) dk = \frac{3}{7} \int_0^1 K(k)^2 K'(k) \frac{dk}{1+k} \end{aligned} \quad (7.50)$$

where the last three integrals follow from the transformations $k \mapsto k'$, $k \mapsto 2\sqrt{k}/(1+k)$ and partial fractions, respectively.

Further work along the same lines of inquiry as [212] produces another proof of (7.37). \diamond

The other integral of a cubic we consider in [169] is

$$\int_0^1 \frac{K'(x)^3}{\sqrt{x}(1-x^2)^{3/4}} dx = \frac{3\Gamma^8(\frac{1}{4})}{32\sqrt{2}\pi^2}. \quad (7.51)$$

To prove (7.51), we use the same procedure to convert the integral into an L -value of a modular form; this time it is $192L(h, 4)$ where

$$h(\tau) := \frac{\eta^{38}(8\tau)}{\eta^{14}(4\tau)\eta^{14}(16\tau)}.$$

The q -expansion for h is found experimentally to be

$$\frac{1}{2} \sum_{m,n=-\infty}^{\infty} (-1)^m (2n+1-2im)^4 q^{(2m)^2+(2n+1)^2}.$$

Once found, this can be proven by standard methods, for instance by using the derivatives of $\theta_2(q^4)$ and $\theta_4(q^4)$. Therefore, we are reduced to showing

$$\sum_{m,n=-\infty}^{\infty} \frac{(-1)^m}{(2n+1+2im)^4} = \frac{\Gamma^8(\frac{1}{4})}{1024\sqrt{2}\pi^2}. \quad (7.52)$$

This can be achieved by elementary sum manipulations of (7.46); indeed, we get

$$\sum_{m,n} \frac{(-1)^m}{(2n+1+m\tau)^4} = \frac{1}{60} (g_2(\tau/2) - 18g_2(\tau) + 32g_2(2\tau)). \quad (7.53)$$

Now (7.52) follows from (7.53) by using $\tau = 2i$ and the 1st, 4th and 16th singular values [46]. Therefore (7.51) is true. We have in fact found explicit evaluations of integrals containing higher powers of K' in [169].

We collect some more results from [169]. It is proven there that for $\tilde{g}(\tau) = \eta^3(r\tau)\eta^3(s\tau)$, where $r + s \equiv 0 \pmod{8}$,

$$L(\tilde{g}, 2) = \frac{8}{\sqrt{rs^3}} k_{r/s} k'_{r/s} K^2(k_{r/s}), \quad (7.54)$$

where, as usual, k_p denotes the p th singular value. Therefore, with $r = 4, s = 4$ or $r = 6, s = 2$, we produce closed forms for the critical L -values of those odd weight modular forms. In the second case, we can convert the η product in terms of elliptic integrals, thus obtaining the evaluation

$$L(\tilde{g}, 2) = \int_0^1 (3 + 6p)^{-\frac{1}{2}} K\left(\frac{p^{\frac{3}{2}}(2+p)^{\frac{1}{2}}}{(1+2p)^{\frac{1}{2}}}\right) dp = \frac{\Gamma^6(\frac{1}{3})}{2^{\frac{17}{3}}\pi^2},$$

where we have used the parametrisation of the degree 3 modular equation and multiplier (see (10.22)). This equation, after a change of variable, has already appeared in a very different context as (2.42) in random walks.

Another connection with random walks is given by the modular form $\tilde{h}(\tau) = \eta^3(3\tau)\eta^3(5\tau) + \eta^3(\tau)\eta^3(15\tau)$. While (7.54) is able to produce closed forms for $L(\tilde{h}, 2)$ and $L(\tilde{h}, 1)$ with little difficulty, we see that equation (3.69) connects $L(\tilde{h}, 4)$ with the Mahler measure $W'_5(0)$. This is a non-critical L -value and so (3.69) is believed to be hard.

Using the multiplicativity of the coefficients of these η products, we are able to rewrite some L -values as conditionally convergent lattice sums; therefore we obtain new results such as

$$\sum'_{m,n} (-1)^{m+1} \frac{m^2 - 2n^2}{(m^2 + 2n^2)^2} = \frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{48\pi}, \quad (7.55)$$

$$\sum'_{m,n} (-1)^{m+n+1} \frac{m^2 - 3n^2}{(m^2 + 3n^2)^2} = \frac{\Gamma^6(\frac{1}{3})}{2^{\frac{14}{3}}\pi^2}, \quad (7.56)$$

$$\sum'_{m,n} (-1)^{m+1} \frac{m^2 - 4n^2}{(m^2 + 4n^2)^2} = \frac{\Gamma^4(\frac{1}{4})}{32\pi}. \quad (7.57)$$

The last two sums correspond to the $r = 4$ and $r = 6$ cases outlined above; for a proof of the first one, we refer to the next section.

Example 7.9.1. As Conjecture 6.2 is fully proven, we may uncouple some of the integrals produced by Legendre's relation in Chapter 6 to give some new closed

forms; they are:

$$\begin{aligned} \int_0^1 E'(x)K(x)K'(x) dx &= \frac{\pi^3}{24} + \frac{\Gamma^8(\frac{1}{4})}{768\pi^2}, & \int_0^1 E(x)K(x)K'(x) dx &= \frac{\pi G}{3} + \frac{\Gamma^8(\frac{1}{4})}{576\pi^2}, \\ \int_0^1 E'(x)K(x)^2 dx &= \frac{2\pi G}{3} + \frac{\Gamma^8(\frac{1}{4})}{1152\pi^2}, & \int_0^1 E(x)K'(x)^2 dx &= \frac{\pi^3}{12} + \frac{\Gamma^8(\frac{1}{4})}{384\pi^2}. \end{aligned} \tag{7.58}$$

◇

Finally, we note that Y. Zhou, in a 2013 preprint [203], used methods based on spherical harmonics to prove both Conjecture 6.2 and equation (7.37).

7.10. Some hypergeometric identities

7.10.1. A hypergeometric transform. We consider the integral

$$\int_0^1 \frac{x}{1+x^2} K(x) dx. \tag{7.59}$$

To evaluate (7.59), we could use the transform $x \mapsto x'$; or, we could apply a quadratic transform followed by a change of variable. In either case, we complete the calculation by interchanging the order of summation and integration, then appeal to the closed form for the moments of K' . The two answers obtained must be the same, and therefore we get the interesting identity

$${}_3F_2\left(\begin{matrix} 1, 1, 1 \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| \frac{1}{2}\right) + {}_3F_2\left(\begin{matrix} 1, 1, 1 \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| -1\right) = \sqrt{2\pi} \Gamma^2\left(\frac{5}{4}\right). \tag{7.60}$$

Along the way we obtain

$$\int_0^1 \frac{x}{1+x^2} K(x) dx = \frac{1}{2} {}_3F_2\left(\begin{matrix} 1, 1, 1 \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| \frac{1}{2}\right), \quad \int_0^1 \frac{1+x}{1+x^2} K(x) dx = \sqrt{2\pi} \Gamma^2\left(\frac{5}{4}\right),$$

c. f. the $t = -1$ case in (7.22).

It is observed that the ${}_3F_2$ above can also be written with argument 1. This suggests the transform

$${}_3F_2\left(\begin{matrix} 1, 1, 1 \\ \frac{3}{2}, 1+2v \end{matrix} \middle| \frac{1}{2}\right) = {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, 1 \\ \frac{3}{2}, 1+v \end{matrix} \middle| 1\right). \tag{7.61}$$

PROOF OF (7.61). Using the beta integral (as is done in the proof of Theorem 5.2), the left hand side of (7.61) can be written as

$$\int_0^1 \frac{8v(1-x^2)^{2v-1}}{\sqrt{2-x^2}} \sin^{-1}\left(\frac{x}{\sqrt{2}}\right) dx.$$

We apply the formula $2 \sin^{-1}(x) = \sin^{-1}(2x\sqrt{1-x^2})$ to this integral, followed by a change of variable, leading to the equivalent integral

$$\int_0^1 2v(1-x^2)^{v-1} \sin^{-1}(x) dx,$$

which is the beta integral for the right hand side of (7.61). \square

7.10.2. Hypergeometric evaluations. We return to (7.35) and (7.55). Denote $I_1 := \int_0^1 \frac{K(x)}{\sqrt{1+x}} dx$; using the moments of K' , we have

$$\int_0^1 \frac{K(x)}{\sqrt{1+x}} dx = \frac{1}{\sqrt{2}} \int_0^1 \frac{K'(x)}{\sqrt{1+x}} dx = \frac{1}{2\sqrt{2}} \left[\frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{16\pi} - {}_4F_3 \left(\begin{matrix} \frac{3}{4}, 1, 1, \frac{5}{4} \\ \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1 \right) \right]. \quad (7.62)$$

Similarly, we have $I_2 :=$

$$\int_0^1 \frac{K(x)}{\sqrt{x(1+x)}} dx = \frac{1}{\sqrt{2}} \int_0^1 \frac{K'(x)}{\sqrt{1-x}} dx = \frac{1}{2\sqrt{2}} \left[\frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{16\pi} + {}_4F_3 \left(\begin{matrix} \frac{3}{4}, 1, 1, \frac{5}{4} \\ \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1 \right) \right]. \quad (7.63)$$

We experimentally observe that (7.63) evaluates to twice the value of (7.62), which we now prove.

It is known that $I_1/(2\sqrt{2}) = L(f_1, 2)$, where $f_1(\tau) = \eta^2(\tau)\eta(2\tau)\eta(4\tau)\eta^2(8\tau)$, and f_1 may be written as $\frac{1}{2} \sum'_{n,m} (m^2 - 2n^2)q^{m^2+2n^2}$ for small $q \geq 0$. Thus, as a lattice sum, I_1 can be obtained by summing over expanding ellipses $m^2+2n^2 \leq M$, $M \rightarrow \infty$ (the convergence here is rather subtle and relies on the convergence of L -values of modular forms):

$$I_1 = \sqrt{2} \sum'_{m,n} \frac{m^2 - 2n^2}{(m^2 + 2n^2)^2}.$$

On the other hand, it can be verified that $I_2/(2\sqrt{2}) = L(f_2, 2)$, where $f_2(q) := -f_1(-q)$ (this comes from the changing $\sqrt{1+x}$ in the denominator to $\sqrt{1-x}$). Consequently, we have

$$I_2 = \sqrt{2} \sum'_{m,n} (-1)^{m+1} \frac{m^2 - 2n^2}{(m^2 + 2n^2)^2}.$$

Now, the lattice sum for $I_2 - I_1$ simplifies to I_1 . Therefore,

$$I_2 = 2I_1, \quad (7.64)$$

as claimed. This result may be arrived at without passing to lattice sums, as we can look at the q -expansion of $f_2 - f_1$ and use the fact that the coefficients of f_1 (being a Hecke eigenform) are multiplicative [143].

A number of results now follow. By using (7.62), (7.63) and (7.64), we have

$${}_4F_3\left(\begin{matrix} \frac{3}{4}, 1, 1, \frac{5}{4} \\ \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) = \frac{\Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{48\pi} = \sqrt{2} I_1 = \frac{1}{\sqrt{2}} I_2, \quad (7.65)$$

and equations (7.35) and (7.55) are now proven.

Remark 7.10.1. Moreover, we also have

$$\sqrt{2} I_1 = \frac{2\pi}{3} {}_4F_3\left(\begin{matrix} \frac{1}{8}, \frac{3}{8}, \frac{1}{2}, \frac{1}{2} \\ 1, \frac{9}{8}, \frac{11}{8} \end{matrix} \middle| 1\right) = \frac{1}{2} \int_0^1 \frac{K(x)}{x^{3/4}} dx - \frac{1}{2} \int_0^1 \frac{K(x)}{x^{1/4}} dx. \quad (7.66)$$

The second equality in (7.66) follows by a contiguous relation and the formulas for the moments of K ; the first equality can be shown by using the Fourier trick (7.42) on the integral definition of I_1 .

In fact, in (7.66), the ratio between the two integrals is $\frac{3\sqrt{2}+2}{3\sqrt{2}-2}$, or equivalently,

$$\int_0^1 \frac{K(x)}{x^{3/4}} dx = 2\pi {}_3F_2\left(\begin{matrix} \frac{1}{8}, \frac{1}{2}, \frac{1}{2} \\ 1, \frac{9}{8} \end{matrix} \middle| 1\right) = {}_3F_2\left(\begin{matrix} \frac{7}{8}, 1, 1 \\ \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| 1\right) = \frac{(2 + 3\sqrt{2}) \Gamma^2(\frac{1}{8})\Gamma^2(\frac{3}{8})}{96\pi}. \quad (7.67)$$

The last equality follows from a generalisation of Saalschütz's theorem [25, §3.8, eqn. (2)]. We start with the first ${}_3F_2$ in (7.67) and apply said generalisation; the result is a ratio of Γ terms plus another ${}_3F_2$. We apply Thomae's transformation [25, p. 14] to this ${}_3F_2$ and find it to be some Γ factors times the ${}_3F_2$ for $\int_0^1 \frac{K(x)}{x^{1/4}} dx$. The desired equality follows by using (7.65) and (7.66) (the $\sqrt{2}$ is due to $\cos \frac{\pi}{4}$ appearing in the calculations).

A neat consequence following from (7.67) is

$$\int_0^1 \left(\frac{x}{x'}\right)^{\frac{1}{2} \pm \frac{1}{4}} K(x) dx = \frac{\pi^2}{12} \sqrt{5 \pm \frac{1}{\sqrt{2}}}, \quad (7.68)$$

after applying Thomae's transformation. \diamond

CHAPTER 8

Elementary Evaluations of Mahler Measures

ABSTRACT. In this chapter, we advocate the use of a trigonometric version of Jensen's formula, and demonstrate its versatility in giving an evaluation and a functional equation for a two-dimensional Mahler measure, and in reducing a three-dimensional measure to a computable integral. We then prove two conjectures of Boyd. We also record some basic facts about Mahler measures, and list some Jensen-like integrals.

8.1. Jensen's formula and Mahler measures

In Section 3.6, we used the formula

$$\int_0^1 \log(a + b \cos(2\pi x)) dx = \log \frac{a + \sqrt{a^2 - b^2}}{2}, \quad a \geq |b| \quad (8.1)$$

to give a very quick evaluation of $W'_3(0)$, recovering a classical result of Smyth. We sketch a proof of equation (8.1) here.

PROOF OF (8.1). It is in fact sufficient to prove the formula for $a = 1$. Differentiating the left hand side of (8.1) with respect to b , the resulting integral is elementary:

$$\int_0^1 \frac{\cos(2\pi x)}{1 + b \cos(2\pi x)} dx = \frac{1}{b} - \frac{1}{b\sqrt{1 - b^2}}.$$

Integrating both sides with respect to b , we obtain

$$\int_0^1 \log(a + b \cos(2\pi x)) dx = \log(1 + \sqrt{1 - b^2}) + C,$$

where C is a constant to be determined. Setting $b = 1$, this integral reduces to

$$\int_0^1 \log(2 \cos^2(\pi x)) dx = C.$$

In order to conclude that $C = -\log 2$, we are required to show

$$\int_0^{\pi/2} \log \cos x dx = -\frac{\log(2)\pi}{2}.$$

Even though this is equivalent to the easy result that $\text{Ls}_2(\pi) = 0$ in the notation of Chapter 9, we prove it here. We have

$$\frac{\pi}{2}C = \int_0^{\pi/2} \log \cos x \, dx = \int_0^{\pi/2} \log \sin x \, dx,$$

so by adding the two integrals, we get

$$\pi C = \int_0^{\pi/2} \log \frac{\sin(2x)}{2} \, dx.$$

By a change of variable we have

$$\pi C = \frac{1}{2} \int_0^{\pi} \log \sin x \, dx - \frac{\log(2)\pi}{2}.$$

However the last integral is πC by symmetry, therefore $\pi C = \pi C/2 - \log(2)\pi/2$ and we are done. \square

Remark 8.1.1. By the identity $a \sin^2 t + b \cos^2 t = \frac{1}{2}((a+b) - (a-b) \cos 2t)$, an equivalent formulation of (8.1) is

$$\int_0^{\pi/2} \log(a \sin^2 t + b \cos^2 t) \, dt = \pi \log \frac{\sqrt{a} + \sqrt{b}}{2}. \quad (8.2)$$

We record a different proof [68] for (8.2):

Denote the integral by $F(a, b)$. Adding $F(a, b)$ to $F(b, a)$ and using symmetry, we obtain $2F(a, b) = F((\frac{a+b}{2})^2, ab)$.

Now consider the iteration

$$x_{n+1} = \frac{(x_n + y_n)^2}{4}, \quad y_{n+1} = x_n y_n, \quad \text{with } x_0 = x, \quad y_0 = y.$$

If we write $a_n = (\sqrt{x_n} + \sqrt{y_n})/2$, $b_n = (\sqrt{x_n} - \sqrt{y_n})/2$, and $d_n = b_n/a_n$, then it is easy to check that $d_{n+1} = d_n^2$ and $0 \leq d_n < 1$. Thus, $y_n/x_n = (1 - d_n)^2/(1 + d_n)^2 \rightarrow 1$.

Hence, $F(x, y) = 2^{-n}F(x_n, y_n) = \pi 2^{-n} \log \sqrt{x_n} + 2^{-n}F(1, y_n/x_n)$ from the integral. From the limit we just established, the second term approaches 0 as $n \rightarrow \infty$. For the first term, since $a_{n+1} = a_n^2$, the limit is found to be $\lim_{n \rightarrow \infty} \pi 2^{-n} \log a_n = \pi \log a_0 = \pi \log((\sqrt{x} + \sqrt{y})/2)$. \diamond

It is not hard to deduce from (8.1) the slightly more general formula, valid for real $|a| \geq |b| > 0$,

$$\int_0^1 \log |2a + 2b \cos(2\pi x)| \, dx = \log(|a| + \sqrt{a^2 - b^2}). \quad (8.3)$$

Formula (8.3) can be thought of as a trigonometric version of *Jensen's formula*, which is commonly written as

$$\int_0^1 \log |a - e^{2\pi it}| dt = \max(\log |a|, 0), \quad (8.4)$$

and indeed can be proven from (8.3). From a psychological viewpoint, it seems to be the case that (8.3) may be used more efficiently or creatively than Jensen's formula, and many Mahler measures can be simplified this way, as we illustrate in this chapter.

Remark 8.1.2 (Related formulas). A range of integrals related to (8.1) can be found. In Chapter 3 we already encountered

$$\int_0^1 \log ((a + \cos 2\pi x)^2 + (b + \sin 2\pi x)^2) dx = \begin{cases} \log(a^2 + b^2) & \text{if } a^2 + b^2 > 1, \\ 0 & \text{otherwise.} \end{cases}$$

This can be proven by expanding the squares in the integrand, writing the sum of sin and cos as a single cos term, then appealing to periodicity and finally to (8.1).

Likewise, we can compute

$$\begin{aligned} & \int_0^1 ((a + \cos 2\pi x)^2 + (b + \sin 2\pi x)^2) \log((a + \cos 2\pi x)^2 + (b + \sin 2\pi x)^2) dx \\ &= \begin{cases} 2 + (a^2 + b^2 + 1) \log(a^2 + b^2) & \text{if } a^2 + b^2 > 1, \\ 2(a^2 + b^2) & \text{otherwise.} \end{cases} \end{aligned}$$

We also have

$$\int_0^1 \begin{Bmatrix} \cos \\ \sin \end{Bmatrix} (2\pi x) \log((a + \cos 2\pi x)^2 + (b + \sin 2\pi x)^2) dx = \frac{\begin{Bmatrix} a \\ b \end{Bmatrix}}{\max(a^2 + b^2, 1)}.$$

The integrals below may be proven by differentiating under the integral sign:

$$\int_0^1 \cos(2\pi x) \log(a + b \cos 2\pi x) dx = \int_0^1 \sin(2\pi x) \log(a + b \sin 2\pi x) dx = \frac{a - \sqrt{a^2 - b^2}}{b},$$

while on the other hand, symmetry dictates that

$$\int_0^1 \sin(2\pi x) \log(a + b \cos 2\pi x) dx = \int_0^1 \cos(2\pi x) \log(a + b \sin 2\pi x) dx = 0.$$

An integral similar to Jensen's formula is

$$\int_0^{2\pi} \log |a + e^{it}| e^{it} dt = \begin{cases} \frac{\pi}{a} & \text{if } |a| \geq 1, \\ \pi a & \text{if } |a| < 1. \end{cases}$$

And finally, we record that

$$\int_0^{1/4} \frac{\log(1 + b \cos 2\pi x)}{\cos 2\pi x} dx = \frac{\pi}{16} - \frac{a \cos^2 b}{4\pi}.$$

◇

8.1.1. Mahler measures. For k Laurent polynomials in n variables, the *multiple Mahler measure*, introduced in [126], is defined as

$$\mu(P_1, P_2, \dots, P_k) := \int_0^1 \cdots \int_0^1 \prod_{j=1}^k \log |P_j(e^{2\pi i t_1}, \dots, e^{2\pi i t_n})| dt_1 dt_2 \dots dt_n. \quad (8.5)$$

When $P = P_1 = P_2 = \dots = P_k$ this devolves to a *higher Mahler measure*, $\mu_k(P)$, also examined in [126]. When $k = 1$ both reduce to the standard (logarithmic) *Mahler measure* [60], which we encountered in Section 3.6.

An easy consequence of Jensen's formula is that for complex constants a and b ,

$$\mu(ax + b) = \max(\log |a|, \log |b|). \quad (8.6)$$

Therefore, the Mahler measure of a monic, single variable polynomial equals $\sum_i \log |r_i|$, where r_i are the roots outside the unit disc. Note that by reversing the coefficients of a polynomial p , the Mahler measure does not change; thus $\mu(P)$ is also equal to $\log |P(0)| - \sum_i \log |s_i|$, where s_i are the roots inside the unit disc. Sometimes the exponential Mahler measure is used, defined by

$$M(P) = e^{\mu(P)},$$

and so $M(P)$ is the product of the roots outside the unit circle. Note that M is multiplicative.

We give some basic facts about the Mahler measures of a single variable polynomial, since they are of historical and continuing interest. Let P be such a polynomial; let L denote the sum of absolute values of the coefficients of P , H be the size of the largest coefficient and d be its degree, then it is well known that [139]

$$M(P) \leq L \leq 2^d M(P).$$

The second inequality follows by using Jensen's formula and expressing the coefficients in terms of the roots, giving $|c_k| \leq \binom{d}{k} M$, where c_k is the k th coefficient of P . Mahler [139] also showed that

$$H2^{-d} \leq M(P) \leq H\sqrt{d+1}.$$

Jensen's formula implies that the Mahler measure of a cyclotomic polynomial is 0, and that the exponential measure of an integer polynomial is an algebraic number.

Kronecker showed that if the Mahler measure of a monic integer polynomial is 0 (that is, if all roots lie in the unit disc), then every root is either 0 or a root of unity. The proof uses invariance under automorphisms of the splitting field and the pigeon hole principle.

A famous open problem involving Mahler measures is as follows. D. H. Lehmer investigated $\Delta_n(P) = \prod_{i=1}^r (a_i^n - 1)$, where a_i are the roots of a monic integer polynomial P . Δ_n is an integer; moreover, when n is a prime, Δ_n may be a large prime whose primality may be checked relatively easily. If we wish for Δ_n to grow slowly with respect to n , that is, we want $\lim_{n \rightarrow \infty} |\Delta_{n+1}/\Delta_n|$ to be small, then it transpires that the $\mu(P)$ needs to be small. This motivates Lehmer's problem (1933) (see e. g. [59]): find the integer polynomial with the smallest non-zero Mahler measure. Note that $x^3 - x - 1$ has small measure, though the current winner is the polynomial

$$x^{10} - x^9 + x^7 - x^6 + x^5 - x^4 + x^3 - x + 1.$$

8.1.2. Multiple Mahler measures. There is much intrinsic interest in studying multiple Mahler measures. For instance, using expansions of algebraic functions, Boyd and Lawton showed that [60]

$$\lim_{n \rightarrow \infty} \mu(P(x, x^n)) = \mu(P(x, y)),$$

(a similar result is true in higher dimensions), so every multiple measure is the limit of one dimensional measures. Another general, deep and difficult connection is with L -series. Loosely speaking, in some cases when a two-variable polynomial whose zero set defines a genus-one curve C , its Mahler measure corresponds to a rational multiple of an L -value of the (modular) elliptic curve arising from C [60, 84]. In a way this 'generalises' Jensen's formula, since in one dimension the L -series at argument 1 evaluates in terms of logarithms, so for two dimensions we may expect the measure to be the L -series at 2 – see e. g. Theorem 8.1. (We briefly looked at some L -values in Chapter 7.)

In physics, multiple Mahler measures occur as certain lattice sums or constants associated with lattices [111, 170].

We now look at some simple techniques for evaluating multiple Mahler measure [181]. An important observation is the following: if there exists an a_j with $|a_j| \geq \sum_{i \neq j} |a_i|$, then by Jensen's formula, we have

$$M(a_0 + a_1x_1 + \cdots + a_nx_n) = a_j. \quad (8.7)$$

(Recall that $M = e^\mu$.) We also note trivially that switching the sign of any of the a_i corresponds to a translation in the integral, and does not change the measure.

From (8.7), we have for instance

$$\begin{aligned} M((x+y)^2 + k) &= k, & k \geq 4, \\ M(a+x+y) &= a, & a \geq 2, \\ M(x^2 - y^2 + xy + 3x - y + 1) &= \phi^2, & \phi = \frac{\sqrt{5}+1}{2}, \end{aligned} \quad (8.8)$$

the last being true since the polynomial factorises as $(x + \phi y + \phi^2)(x - y/\phi + 1/\phi^2)$.

Another fundamental principle is to notice that the two dimensional Mahler measure is an integral over a torus, so if for functions F and G ,

$$G(x, y) = F(x^a y^b, x^c y^d), \quad ad - bc = 1,$$

then $\mu(G) = \mu(F)$. This is because the change of variables $(x, y) \mapsto (ax+by, cx+dy)$ has Jacobian 1, and takes the unit square to another fundamental domain of the torus. (This periodicity idea is used in e.g. Section 4.2, and also in this chapter.)

A third basic technique for finding multiple Mahler measures is to apply Jensen's formula creatively – by writing the polynomial as $A + yB$ where A and B do not depend on y . For instance, Smyth's original evaluation of $\mu(1+x+y+z)$ starts by writing it as $\mu((1+x) + y(1+z/y)) = \mu(\max(|1+x|, |1+z|))$, by a change of variable and Jensen's formula (8.4). Often Jensen's formula needs to be applied multiple times.

This technique easily leads to $\mu(1+xy) = 0$, as well as

$$\mu(1+x+y-xy) = \frac{2G}{\pi}, \quad \mu(1+x+x^2+y) = \frac{8G}{3\pi}, \quad \mu(1+x+y+x^2y) = \frac{3\text{Cl}(\frac{\pi}{3})}{\pi}, \quad (8.9)$$

where G denotes Catalan's constant and Cl is the Clausen function.

We give here a slight modification to the above approach, which is to use formula (8.3) instead. The procedure is to write the integrand as a trigonometric expression, which allows us to apply sum-to-product and product-to-sum formulas (including

double angle formulas) liberally. Combined with translations which are allowed due to periodicity, our aim is to ‘isolate’ a variable (y) so that (8.3) can be applied. Although this method is by no means a panacea, it does have its advantages. We get more freedom and control over the manipulations, and computers can be used to automate (or exhaust) our searches, which are often non-trivial as there are often many ways to group different trigonometric terms together, or to split them up. Moreover, we often succeed in completing a one- or two-dimensional reduction; the resulting integrals often appear as log-sine integrals (Chapter 9), or are at least amenable to numerical integration. All of the measures in (8.9) can be done with this method with great ease. We will apply these methods below, especially in Section 8.4.

Example 8.1.1. We apply (8.3) to the Mahler measure $\mu(a + x + y)$.

First note that the $a > 2$ case has been dealt with in (8.8). Write μ using its definitional integral. The integrand inside the log simplifies to

$$2 + a^2 + 4a \cos(\pi(x - y)) \cos(\pi(x + y)) + 2 \cos(2\pi(x - y)).$$

Using the change of variable $u = x - y, v = x + y$ and symmetries in the region of integration, we are able to apply (8.3) to deduce that for $a = 2 \sin(s/2)$ and $s \in (0, \pi)$,

$$\mu(a + x + y) = \int_0^{(\pi-s)/(2\pi)} 2 \log(2 \cos \pi u) \, du + \frac{s \log 2(1 - \cos s)}{2\pi},$$

which simplifies to

$$\mu\left(2 \sin \frac{s}{2} + x + y\right) = \frac{1}{\pi} \left(\text{Cl}(s) + s \log \left(2 \sin \frac{s}{2}\right) \right). \quad (8.10)$$

Moreover, combined with (8.4) and the fact that $\max\{|x^n|, |y^n|\} = \max\{|x|, |y|\}^n$, we obtain

$$\mu\left(\left(2 \sin \frac{s}{2}\right)^n + (x + y)^n\right) = \frac{n}{\pi} \left(\text{Cl}(s) + s \log \left(2 \sin \frac{s}{2}\right) \right).$$

The exact result by Cassaigne-Maillot [141] for $\mu(a + bx + cy)$ can also be deduced in the same way. \diamond

An asymptotic expansion for the Mahler measure $\mu(1 + x_1 + \cdots + x_n)$ is given in Section 4.3.

8.2. On $\mu(k + x + 1/x + y + 1/y)$

We give an independent and elementary evaluation of the Mahler measure

$$\mu_k := \mu(k + x + 1/x + y + 1/y).$$

This measure is considered in [167], and many of its properties have been rediscovered several times. It has been pointed out to us that our main results, equations (8.15) and (8.16), were first found in [127].

Nevertheless, our analysis was carried out without any knowledge of previous work, and due to its brevity we record it below. As outlined in the last section, we first convert the exponentials in the double integral of μ_k into trigonometric functions, so we are reduced to computing

$$\mu_k = \int_0^1 \int_0^1 \log |k + 2 \cos(2\pi x) + 2 \cos(2\pi y)| \, dx dy.$$

We do not apply (8.3) yet. Upon writing the sum of cosines as a product, we obtain the equivalent formula

$$\mu_k = \int_0^1 \int_0^1 \log |k + 4 \cos(\pi(x - y)) \cos(\pi(x + y))| \, dx dy.$$

Now make the change of variable $x - y = u$, $x + y = v$, appeal to periodicity and apply the trigonometric version of Jensen's formula (8.3). (This change of variable corresponds to the equality $\mu(k + x + 1/x + y + 1/y) = \mu(k + (x + 1/x)(y + 1/y))$.)

After cleaning up the $|\cdot|$ in the resulting single integral, we obtain

$$\mu_k = \int_0^1 \log \left| \frac{k}{2} + \sqrt{\frac{k^2}{4} - 4 \cos^2 \pi u} \right| \, du. \quad (8.11)$$

We consider the two cases, $k \geq 4$ and $k \leq 4$. If $k \geq 4$, then we may disregard the $|\cdot|$ in (8.11). After a trigonometric change of variable, we obtain

$$\mu_k = \frac{1}{\pi} \int_0^1 \frac{\log \left(1 + \sqrt{1 - \frac{16t}{k^2}} \right)}{\sqrt{t(1-t)}} \, dt + \log \frac{k}{2}.$$

We can legally expand the log as a series, exchange the order of summation and integration, and observe that the integral gives a ${}_2F_1$. Writing that as a series, we then interchange the order of summation, and arrive at the closed form

$$\mu_k = \log k - \frac{2}{k^2} {}_4F_3 \left(\begin{matrix} 1, 1, \frac{3}{2}, \frac{3}{2} \\ 2, 2, 2 \end{matrix} \middle| \frac{16}{k^2} \right), \quad k \geq 4. \quad (8.12)$$

If, on the other hand, $k \leq 4$, then the absolute value in (8.11) splits the integral into two parts, which give

$$\pi \mu_k = \text{Cl}\left(2 \sin^{-1} \frac{k}{4}\right) + 2 \sin^{-1}\left(\frac{k}{4}\right) \log\left(\frac{k}{2}\right) + \frac{k}{4} \int_0^1 \frac{\log(1 + \sqrt{1-t})}{\sqrt{t(1 - \frac{k^2 t}{16})}} dt. \quad (8.13)$$

We apply the same tricks as in the $k \geq 4$ case above to treat the last integral. One additional detail we need to take care of is that, after the second exchange of summation, we split up the inner sum over even and odd terms. The result is the sum of two hypergeometric functions:

$$\pi {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{k^2}{16}\right) - 2 {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{k^2}{16}\right).$$

We now observe that one ${}_3F_2$ above cancels with the first two terms in (8.13) by equation (3.62); thus we have

$$\mu_k = \frac{k}{4} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{k^2}{16}\right) = \frac{2}{\pi} \int_0^{\frac{k}{4}} K(x) dx, \quad k \leq 4. \quad (8.14)$$

Note that at $k = 4$, we obtain the reduction (c. f. (5.32))

$$\mu_4 = \frac{4G}{\pi}.$$

Moreover, by inverting the argument of the ${}_3F_2$ in (8.12) using equation (3.31), we obtain

Theorem 8.1. For $k \geq 0$,

$$\mu_k = \frac{k}{4} \text{Re} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| \frac{k^2}{16}\right). \quad (8.15)$$

The identification of μ_k with the real part of incomplete moments of K , as in (8.14), allows us to find linear relations for various values of k . For instance, if we start with μ_5 , apply Jacobi's imaginary transformation followed by the quadratic transform (6.5), then we are able to split it into two Mahler measures; that is,

$$\mu_5 = \frac{2}{\pi} \left(2G + \int_{\frac{4}{5}}^1 \frac{K(x)}{x} dx\right) = \frac{1}{\pi} \left(2G + \int_{\frac{1}{4}}^1 \frac{K(x)}{x} dx\right) + \frac{1}{\pi} \left(2G - \int_{\frac{1}{4}}^1 K(x) dx\right).$$

Identifying each piece using (8.14) and some transforms, the end result is

$$2\mu_5 = \mu_1 + \mu_{16}.$$

Indeed, this method in general gives the functional equation

$$\mu_{4k^2} + \mu_{4/k^2} = 2\mu_{2k+2/k}, \quad (8.16)$$

therefore, the last formula corresponds to the $k = 2$ case; another visually pleasing case is $\mu_2 + \mu_8 = 2\mu_{3\sqrt{2}}$.

Unfortunately, (8.16) does not resolve Boyd's observations that $\mu_8 = 4\mu_2$ and $\mu_5 = 6\mu_1$, which are proved in [129] and [128] respectively.

We remark that μ_1 was conjectured by Deninger to evaluate as

$$\mu(1 + x + y + 1/x + 1/y) = \frac{15}{4\pi^2} L(f, 2), \quad (8.17)$$

where $f(\tau) = \eta(\tau)\eta(3\tau)\eta(5\tau)\eta(15\tau)$. The conjecture has recently been proven in [170].

8.3. On $\mu((1+x)(1+y)+z)$.

In this section, we provide strong numerical evidence for a conjecture by Boyd, who also numerically validated it to 28 digits by an illustrative use of the Cassaigne-Maillot formula; the history is given in [61]. Let $P = (1+x)(1+y)+z$, and let $\mu^* := \mu(P)$. The conjecture is

$$\mu^* \stackrel{?}{=} 2L'(E_N, -1) = \frac{4N^2}{(2\pi)^4} L(E_N, 3), \quad (8.18)$$

where E_N is the elliptic curve of conductor (see e.g. [178]) $N = 15$, defined by $P = 0$, and L is the L -series attached to E_N .

We find an easily integrable one dimensional integral for μ^* . We follow the methods outlined in Section 8.1.2 and proceed via the following steps:

- (1) Write the integrand as trigonometric terms and factorise in such a way that z only appears in one term.
- (2) Now that z is 'isolated', make the change of variable $z - (x+y)/2 \mapsto z$, which is justified by periodicity.
- (3) Apply the trigonometric version of Jensen's formula, (8.3).
- (4) Factorise the expression in the resulting integrand.
- (5) Find the region on which the integrand is positive (and note that it is 0 elsewhere).
- (6) Appeal to symmetry.

Carrying out the first five steps, it is not hard to arrive at

$$\mu^* = \frac{4}{\pi^2} \int_0^{\cos^{-1} \frac{1}{4}} \int_0^{\cos^{-1} \frac{\sec x}{4}} \log(4 \cos(x) \cos(y)) \, dx dy.$$

(E. g. the outcome of steps 1 and 2 is the expression, after a linear change of variable, $5 + 8 \cos(x - y) \cos(x + y) + 4 \cos(2x) \cos(2y) + 8 \cos(x) \cos(y) \cos(2z)$.)

By symmetry of the integration region, we obtain the single integral,

$$\mu^* = \frac{8}{\pi^2} \int_0^{\cos^{-1} \frac{1}{4}} \cos^{-1} \left(\frac{\sec x}{4} \right) \log(2 \cos x) dx = \frac{8}{\pi^2} \int_1^4 \frac{\sec^{-1}(t) \log \frac{t}{2}}{\sqrt{16 - t^2}} dt. \quad (8.19)$$

This procedure works more generally: for $b \in (0, 4)$, we have

$$\mu_b^* := \mu((1+x)(1+y) + bz) = \log(b) + \frac{8}{\pi^2} \int_b^4 \frac{\arccos\left(\frac{b}{x}\right) \log\left(\frac{x}{2\sqrt{b}}\right)}{\sqrt{16 - x^2}} dx. \quad (8.20)$$

Note that for $b \geq 4$, $\mu_b^* = \log(b)$, which is a simple consequence of (8.7).

Even though (8.19) is not a closed form, the integral is very easy to compute numerically. The singularity at 4 is rather mild, and can be removed with a number of quadrature schemes such as tanh-sinh or Gaussian quadrature; we do not explore those here and only mention that Gaussian quadrature is investigated in Chapter 14.

After discovering (8.19), we used it to verify (8.18) to 500 digits in under 3 minutes. The integral was evaluated by running *Mathematica 7* on a modest laptop, using the `NIntegrate` command with increased `WorkingPrecision` and `PrecisionGoal` options, and no other quadrature schemes; the L -series is easy to compute and its digits are in fact well-tabulated. Later (in March 2012) we verified (8.18) to 1000 digits, which took under 30 minutes of computing time.

8.4. Proofs of two conjectures of Boyd

We recapture the following evaluations conjectured by Boyd in 1998 and first proven in [186] using Bloch-Wigner dilogarithms. Below, L_{-n} denotes the primitive L -series mod n .

Theorem 8.1. *We have*

$$\mu(y^2(x+1)^2 + y(x^2 + 6x + 1) + (x+1)^2) = \frac{16}{3\pi} L_{-4}(2) = \frac{16G}{3\pi}, \quad (8.21)$$

as well as

$$\mu(y^2(x+1)^2 + y(x^2 - 10x + 1) + (x+1)^2) = \frac{5\sqrt{3}}{\pi} L_{-3}(2) = \frac{20}{3\pi} \text{Cl}_2\left(\frac{\pi}{3}\right). \quad (8.22)$$

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 $x = e^{2\pi it}$, $y = e^{2\pi iu}$ and note that

$$\begin{aligned} |P_c| &= |(x+1)^2(y^2 + y + 1) + 2(c-1)xy| \\ &= |(x+x^{-1}+2)(y+y^{-1}+1) + 2(c-1)| \\ &= |2(\cos(2\pi t) + 1)(2\cos(2\pi u) + 1) + 2(c-1)| \\ &= 2|c + 2\cos(2\pi u) + (1 + 2\cos(2\pi u))\cos(2\pi t)|. \end{aligned}$$

(This factorisation was discovered experimentally, by first converting $|P_c|$ into trigonometric terms, and then, aided by a computer, by considering the many possible ways to repeatedly combine two of the terms into a single term using the *prosthaphaeresis* formulas.)

Applying (8.3), with $a = c + 2\cos(2\pi u)$ and $b = 1 + 2\cos(2\pi u)$ to $\int_0^1 \log |P_c| dt$, we get

$$\mu_c = \int_0^1 \log \left| c + 2\cos(2\pi u) + \sqrt{(c^2 - 1) + 4(c-1)\cos(2\pi u)} \right| du. \quad (8.23)$$

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 $|a| \geq |b|$.

(a) When $c = 3$ for (8.21), by symmetry, and after factorisations we obtain

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

where for the penultimate equality we have split up the integrand and used a few basic transformations.

(b) When $c = -5$ for (8.22), we likewise obtain

$$\begin{aligned}
\mu_{-5} &= \frac{2}{\pi} \int_0^\pi \log(\sqrt{3} + 2 \sin \theta) \, d\theta = \frac{2}{\pi} \int_{\pi/3}^{4\pi/3} \log(\sqrt{3} + 2 \sin(\theta - \frac{\pi}{3})) \, d\theta \\
&= \frac{2}{\pi} \int_{\pi/3}^{4\pi/3} \left\{ \log 2 \left(\sin \frac{\theta}{2} \right) + \log 2 \left(\sin \frac{\theta + \frac{\pi}{3}}{2} \right) \right\} \, d\theta \\
&= \frac{2}{\pi} \int_{\pi/3}^{4\pi/3} \log 2 \left(\sin \frac{\theta}{2} \right) \, d\theta + \frac{2}{\pi} \int_{2\pi/3}^{5\pi/3} \log 2 \left(\sin \frac{\theta}{2} \right) \, d\theta \\
&= \frac{4}{\pi} \operatorname{Cl}_2 \left(\frac{\pi}{3} \right) - \frac{4}{\pi} \operatorname{Cl}_2 \left(\frac{4\pi}{3} \right) = \frac{20}{3\pi} \operatorname{Cl}_2 \left(\frac{\pi}{3} \right),
\end{aligned}$$

since $\operatorname{Cl}_2 \left(\frac{4\pi}{3} \right) = -\frac{2}{3} \operatorname{Cl}_2 \left(\frac{\pi}{3} \right)$. \square

When $c = 1$ the cosine in the surd of (8.23) disappears, and we obtain $\mu_1 = 0$, which is trivial as in this case the polynomial factorises as $(1+x)^2(1+y+y^2)$. For $c = -1$ we are able to obtain a new Mahler measure evaluation:

Theorem 8.2. *We have*

$$\begin{aligned}
\mu_{-1} &= \mu((x+1)^2(y^2+y+1) - 4xy) \\
&= \frac{\beta(\frac{1}{4}, \frac{1}{4})}{4\pi} {}_3F_2 \left(\frac{1}{4}, \frac{1}{4}, 1 \mid \frac{1}{4} \right) - \frac{\beta(\frac{3}{4}, \frac{3}{4})}{6\pi} {}_3F_2 \left(\frac{3}{4}, \frac{3}{4}, 1 \mid \frac{1}{4} \right).
\end{aligned} \tag{8.24}$$

Here, $\beta(s, t) = \frac{\Gamma(s)\Gamma(t)}{\Gamma(s+t)}$ denotes the Euler beta function.

PROOF. We only sketch the proof here. First, using (8.23) we have

$$\mu_{-1} = \frac{4G}{3\pi} + \frac{4}{\pi} \int_0^1 \frac{x \log(1 + \sqrt{2}x)}{\sqrt{1-x^4}} \, dx.$$

Replacing the $\sqrt{2}$ in the integrand by a , *Mathematica* is able to evaluate the integral in terms of three ${}_3F_2$'s with argument a^4 . For $|a| < 1$, one can show that the evaluation is indeed correct, by writing the ${}_3F_2$'s as Euler-type integrals of ${}_2F_1$'s as done in (5.22). By analytic continuation, the evaluation also holds for $a = \sqrt{2}$; it remains to invert the argument in the ${}_3F_2$'s using (3.31), and to note that one of hypergeometrics cancels with the Catalan constant term. \square

Log-sine Evaluations of Mahler Measures

ABSTRACT. We study higher and multiple Mahler measures using log-sine integrals. This motivates a detailed study of multiple polylogarithms. Our techniques enable the reduction of several multiple Mahler measures.

9.1. Introduction

In [55] the classical log-sine integrals and their extensions are used to develop a variety of results relating to higher and multiple Mahler measures [60, 126]. Log-sine evaluations are used in physics: they appear for instance in the calculation of the ε -expansion of various Feynman diagrams [120]. They also come up in number theory and analysis: classes of inverse binomial sums can be expressed in terms of generalised log-sine integrals [51, 83].

The structure of this chapter is as follows. In Section 9.2 our basic tools and results are described. We turn to relationships between random walks and Mahler measures in Section 9.3. In particular, we will be interested in the multiple Mahler measure $\mu_n(1+x+y)$ which has a hypergeometric generating function (9.22) and a trigonometric representation (9.24) as a double integral.

In Section 9.4 we directly expand (9.22) and use results from the ε -expansion of hypergeometric functions [82, 83] to obtain $\mu_n(1+x+y)$ in terms of multiple inverse binomial sums. For $n = 1, 2, 3$ this leads to explicit polylogarithmic evaluations.

An alternative approach based of the double integral representation (9.24) is taken up in Section 9.5 which considers the evaluation of the inner integral in (9.24). Aided by combinatorics, we show that these can always be expressed in terms of multiple polylogarithms. Accordingly, we demonstrate in Section 9.5.2 how these polylogarithms can be reduced explicitly for low weights. In Section 9.6 we reprise from [55] the evaluation of $\mu_2(1+x+y)$.

9.2. Preliminaries and log-sine integrals

We will need the definition of a multiple Mahler measure (8.5).

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

In the following development, we let

$$\text{Li}_{a_1, \dots, a_k}(z) := \sum_{n_1 > \dots > n_k > 0} \frac{z^{n_1}}{n_1^{a_1} \cdots n_k^{a_k}} \quad (9.1)$$

denote the *generalised polylogarithm* as is studied in [51] and [44, Ch. 3]. For example, $\text{Li}_{2,1}(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2} \sum_{j=1}^{k-1} \frac{1}{j}$. In particular, $\text{Li}_k(x) := \sum_{n=1}^{\infty} \frac{x^n}{n^k}$ is the *polylogarithm of order k*. The dilogarithm function Li_2 [199] has a particularly rich structure.

Moreover, *multiple zeta values* (see Chapter 13) are denoted by

$$\zeta(a_1, \dots, a_k) := \text{Li}_{a_1, \dots, a_k}(1). \quad (9.2)$$

Similarly, we consider the multiple Clausen functions (Cl) and multiple Glaisher functions (Gl) of depth k which are given by

$$\text{Cl}_{a_1, \dots, a_k}(\theta) = \begin{cases} \text{Im Li}_{a_1, \dots, a_k}(e^{i\theta}) & \text{if } w \text{ even} \\ \text{Re Li}_{a_1, \dots, a_k}(e^{i\theta}) & \text{if } w \text{ odd} \end{cases}, \quad (9.3)$$

$$\text{Gl}_{a_1, \dots, a_k}(\theta) = \begin{cases} \text{Re Li}_{a_1, \dots, a_k}(e^{i\theta}) & \text{if } w \text{ even} \\ \text{Im Li}_{a_1, \dots, a_k}(e^{i\theta}) & \text{if } w \text{ odd} \end{cases}, \quad (9.4)$$

where $w = a_1 + \dots + a_k$ is the weight of the function.

For $n = 1, 2, \dots$, we consider the *log-sine integrals* defined by

$$\text{Ls}_n(\sigma) := - \int_0^\sigma \log^{n-1} \left| 2 \sin \frac{\theta}{2} \right| d\theta, \quad (9.5)$$

and, for $k = 0, 1, \dots, n-1$, their generalised versions

$$\text{Ls}_n^{(k)}(\sigma) := - \int_0^\sigma \theta^k \log^{n-1-k} \left| 2 \sin \frac{\theta}{2} \right| d\theta. \quad (9.6)$$

This is the notation used by Lewin [133, 134].

Clearly, $\text{Ls}_1(\sigma) = -\sigma$ and that $\text{Ls}_n^{(0)}(\sigma) = \text{Ls}_n(\sigma)$. In particular,

$$\text{Ls}_2(\sigma) = \text{Cl}_2(\sigma) := \sum_{n=1}^{\infty} \frac{\sin(n\sigma)}{n^2} \quad (9.7)$$

is the Clausen function. In Section 5.3 we proved $\text{Cl}_2(\pi/2) = G$ from the integral definition. Various log-sine integral evaluations may be found in [134, §7.6 & §7.9].

9.2.1. Log-sine integrals at π . Log-sine integrals at π can always be evaluated in terms of zeta values. This is a consequence of the (easy) exponential generating function

$$-\frac{1}{\pi} \sum_{m=0}^{\infty} \text{Ls}_{m+1}(\pi) \frac{u^m}{m!} = \frac{\Gamma(1+u)}{\Gamma^2(1+\frac{u}{2})} = \binom{u}{u/2}. \quad (9.8)$$

This will be revisited in Section 9.3. It is not hard to see from the definition that log-sine integrals at π correspond to higher Mahler measures:

$$\mu_m(1+x) = -\frac{1}{\pi} \text{Ls}_{m+1}(\pi) \quad (9.9)$$

Example 9.2.1 (Values of $\text{Ls}_n(\pi)$). For instance, we have $\text{Ls}_2(\pi) = 0$ as well as

$$\begin{aligned} -\text{Ls}_3(\pi) &= \frac{1}{12} \pi^3 \\ \text{Ls}_4(\pi) &= \frac{3}{2} \pi \zeta(3) \\ -\text{Ls}_5(\pi) &= \frac{19}{240} \pi^5 \\ \text{Ls}_6(\pi) &= \frac{45}{2} \pi \zeta(5) + \frac{5}{4} \pi^3 \zeta(3) \\ -\text{Ls}_7(\pi) &= \frac{275}{1344} \pi^7 + \frac{45}{2} \pi \zeta^2(3) \end{aligned}$$

and so forth. Note that these values may be conveniently obtained from (9.8) by a computer algebra system with a one line command.

Many more results may be obtained from these. For instance, integrating $\text{Ls}_3(\pi)$ by parts, we find

$$\int_0^{\pi} t \cot\left(\frac{t}{2}\right) \log\left(2 \sin \frac{t}{2}\right) dt = \pi \log(2)^2 - \frac{\pi^3}{12}.$$

It is straightforward to see that as $n \rightarrow \infty$, $\text{Ls}_n(\pi) \rightarrow \text{Ls}_n(\pi/3)$. A change of variable in the integral of the latter gives, as $n \rightarrow \infty$,

$$\begin{aligned} \left| \text{Ls}_n\left(\frac{\pi}{3}\right) \right| &= \int_0^{1/2} \frac{2|\log^{n-1}(2x)|}{\sqrt{1-x^2}} dx = \int_0^{1/2} \left(2 + x^2 + \frac{3x^4}{4} + \dots\right) |\log^{n-1}(2x)| dx \\ &= \Gamma(n) \left(1 + \frac{1}{8 \cdot 3^n} + \frac{3}{128 \cdot 5^n} + \dots\right), \end{aligned} \quad (9.10)$$

which gives the asymptotic behaviour of the Mahler measures (9.9) and (9.51) below.

◇

For general log-sine integrals, the following computationally effective exponential generating function was obtained in [54].

Theorem 9.1 (Generating function for $\text{Ls}_{n+k+1}^{(k)}(\pi)$). *For $2|\mu| < \lambda < 1$ we have*

$$\sum_{n,k \geq 0} \text{Ls}_{n+k+1}^{(k)}(\pi) \frac{\lambda^n (i\mu)^k}{n! k!} = -i \sum_{n \geq 0} \binom{\lambda}{n} \frac{(-1)^n e^{i\pi \frac{\lambda}{2}} - e^{i\pi \mu}}{\mu - \frac{\lambda}{2} + n}. \quad (9.11)$$

One may extract one-variable generating functions from (9.11). For instance,

$$\sum_{n=0}^{\infty} \text{Ls}_{n+2}^{(1)}(\pi) \frac{\lambda^n}{n!} = \sum_{n=0}^{\infty} \binom{\lambda}{n} \frac{-1 + (-1)^n \cos \frac{\pi \lambda}{2}}{(n - \frac{\lambda}{2})^2}.$$

9.2.2. Extensions of the log-sine integrals. It is possible to consider the log-sine-cosine integrals

$$\text{Lsc}_{m,n}(\sigma) := - \int_0^\sigma \log^{m-1} \left| 2 \sin \frac{\theta}{2} \right| \log^{n-1} \left| 2 \cos \frac{\theta}{2} \right| d\theta. \quad (9.12)$$

Then $\text{Lsc}_{m,1}(\sigma) = \text{Ls}_m(\sigma)$ and $\text{Lsc}_{m,n}(\sigma) = \text{Lsc}_{n,m}(\sigma)$. As in (9.9), these are related to multiple Mahler measures. Namely, if we set

$$\mu_{m,n}(1-x, 1+x) := \mu(\underbrace{1-x, \dots, 1-x}_m, \underbrace{1+x, \dots, 1+x}_n) \quad (9.13)$$

then, from the definition, we obtain the following:

Theorem 9.2 (Evaluation of $\mu_{m,n}(1-x, 1+x)$). *For non-negative integers m, n ,*

$$\mu_{m,n}(1-x, 1+x) = -\frac{1}{\pi} \text{Lsc}_{m+1,n+1}(\pi). \quad (9.14)$$

In every case this is evaluable in terms of zeta values. Indeed, using the result in [134, (7.114)], we obtain the generating function

$$\text{gs}(u, v) := -\frac{1}{\pi} \sum_{m,n=0}^{\infty} \text{Lsc}_{m+1,n+1}(\pi) \frac{u^m v^n}{m! n!} = \frac{2^{u+v}}{\pi} \frac{\Gamma(\frac{1+u}{2}) \Gamma(\frac{1+v}{2})}{\Gamma(1 + \frac{u+v}{2})}. \quad (9.15)$$

We have

$$\text{gs}(u, 0) = \binom{u}{u/2} = \text{gs}(u, u),$$

so clearly (9.15) is an extension of (9.8).

Example 9.2.2 (Values of $\text{Lsc}_{n,m}(\pi)$). For instance,

$$\begin{aligned}\mu_{1,1}(1-x, 1+x) &= -\frac{\pi^2}{24}, \\ \mu_{2,1}(1-x, 1+x) &= \mu_{1,2}(1-x, 1+x) = \frac{1}{4}\zeta(3), \\ \mu_{3,2}(1-x, 1+x) &= \frac{3}{4}\zeta(5) - \frac{1}{8}\pi^2\zeta(3).\end{aligned}$$

As in Example 9.2.1, these can be easily obtained with a line of code. ◇

Remark 9.2.1. From $\text{gs}(u, -u) = \sec(\pi u/2)$ we may deduce that

$$\sum_{k=0}^n (-1)^k \mu_{k,n-k}(1-x, 1+x) = |E_{2n}| \frac{(\pi/2)^{2n}}{(2n)!} = \frac{4}{\pi} \beta(2n+1),$$

where E_{2n} are the Euler numbers: 1, -1, 5, -61, 1385 . . . , see also Section 13.4. ◇

Using Fourier techniques, one may prove in much the same way as Proposition 9.8 the following result, first given in [126].

Proposition 9.1 (A dilogarithmic measure). *For two complex numbers u and v we have*

$$\mu(1-ux, 1-vx) = \begin{cases} \frac{1}{2} \text{Re Li}_2(v\bar{u}), & \text{if } |u| \leq 1, |v| \leq 1, \\ \frac{1}{2} \text{Re Li}_2\left(\frac{v}{u}\right), & \text{if } |u| \geq 1, |v| \leq 1, \\ \frac{1}{2} \text{Re Li}_2\left(\frac{1}{v\bar{u}}\right) + \log|u| \log|v|, & \text{if } |u| \geq 1, |v| \geq 1. \end{cases} \quad (9.16)$$

In Lewin’s terms [134, A.2.5], we may write the above result in terms of

$$\text{Li}_2(r, \theta) := \text{Re Li}_2(re^{i\theta}) = -\frac{1}{2} \int_0^r \log(t^2 + 1 - 2t \cos \theta) \frac{dt}{t}, \quad (9.17)$$

which satisfies the reflection formula

$$\text{Li}_2(r, \theta) + \text{Li}_2\left(\frac{1}{r}, \theta\right) = \zeta(2) - \frac{1}{2} \log^2 r + \frac{1}{2} (\pi - \theta)^2. \quad (9.18)$$

Example 9.2.3 (Some more evaluations). Since $\text{Cl}_2(t) = \sum_{n>0} \frac{\sin(nt)}{n^2}$, by Parseval’s formula [125] we have

$$\int_0^\pi \text{Cl}_2^2(t) dt = \frac{\pi^5}{180}, \quad (9.19)$$

and integration by parts gives results such as

$$\int_0^\pi t \log\left(2 \sin \frac{t}{2}\right) \text{Cl}(t) dt = \frac{\pi^5}{360}, \quad \int_0^{\pi/2} \log\left(2 \sin \frac{t}{2}\right) \text{Cl}(t) dt = -\frac{G^2}{2}.$$

Moreover, we have the moments

$$\int_0^\pi t^n \text{Cl}(t) dt = \frac{1}{n+1} \text{Ls}_{n+3}^{(n+1)}(\pi).$$

From (9.18), we have

$$\text{Li}_2(e^{it}) = \frac{\pi^2}{6} + \frac{t^2 - 2\pi t}{4} + i \text{Cl}_2(t),$$

thus we may expand out $\text{Li}_2^2(e^{it})$, use the moments above and equation (9.19) to find

$$\int_0^\pi \text{Li}_2^2(e^{it}) dt = \frac{i}{48} (10\pi^2 \zeta(3) - 93\zeta(5)).$$

◇

9.3. Mahler measures and moments of random walks

Recall that the s th moments of an n -step uniform random walk are given by

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

and their relation with Mahler measures is observed in Chapter 3. In particular,

$$W_n'(0) = \mu(1 + x_1 + \cdots + x_{n-1}).$$

Higher derivatives of W_n correspond to higher Mahler measures:

$$W_n^{(m)}(0) = \mu_m(1 + x_1 + \cdots + x_{n-1}). \quad (9.20)$$

The evaluation $W_2(s) = \binom{s}{s/2}$ thus explains and proves the generating function (9.8); in other words, we find that

$$W_2^{(m)}(0) = -\frac{1}{\pi} \text{Ls}_{m+1}(\pi). \quad (9.21)$$

We record the following generating function for $\mu_m(1 + x + y)$ which follows from (9.20) and the hypergeometric expression for W_3 .

Theorem 9.3 (Hypergeometric form for $W_3(s)$). *For complex $|s| < 2$, we may write*

$$W_3(s) = \sum_{n=0}^{\infty} \mu_n(1 + x + y) \frac{s^n}{n!} = \frac{3^{s+3/2}}{2\pi} \frac{\Gamma(1 + \frac{s}{2})^2}{\Gamma(s+2)} {}_3F_2 \left(\begin{matrix} \frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2} \\ 1, \frac{s+3}{2} \end{matrix} \middle| \frac{1}{4} \right) \quad (9.22)$$

$$= \frac{\sqrt{3}}{\pi} \left(\frac{3}{2} \right)^{s+1} \int_0^1 \frac{z^{1+s}}{\sqrt{1-z^2}} {}_2F_1 \left(\begin{matrix} 1 + \frac{s}{2}, 1 + \frac{s}{2} \\ 1 \end{matrix} \middle| \frac{z^2}{4} \right) dz. \quad (9.23)$$

PROOF. Equation (9.22) is a consequence of equation (3.75), while (9.23) is equivalent to (9.22) after interchanging the order of integration and summation and applying a beta integral. \square

By computing higher-order finite differences in the right-hand side of (9.22), we have obtained values for $\mu_n(1+x+y)$ to several thousand digits.

We shall exploit Theorem 9.3 in Section 9.4. We also have

$$\mu_n(1+x+y) = \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_0^{2\pi} (\operatorname{Re} \log(1 - 2\sin(\theta)e^{i\omega}))^n d\omega, \quad (9.24)$$

as follows directly from the definition and simple trigonometry. In Section 9.5 we will evaluate the inner integral in terms of multiple polylogarithms.

9.4. Epsilon expansion of W_3

In this section we use known results from the ε -expansion of hypergeometric functions [82, 83] 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 $\mu_3(1+x+y)$. Alternative approaches will be pursued in Sections 9.5 and 9.6.

In light of Theorem 9.3, the evaluation of $\mu_n(1+x+y)$ is essentially reduced to the Taylor expansion

$${}_3F_2\left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4}\right) = \sum_{n=0}^{\infty} \alpha_n \varepsilon^n. \quad (9.25)$$

Indeed, from (9.22) we have

$$\mu_n(1+x+y) = \frac{\sqrt{3}}{2\pi} \sum_{k=0}^n \binom{n}{k} \alpha_k \beta_{n-k}, \quad (9.26)$$

where β_k is defined by

$$\frac{3^{\varepsilon+1}}{(1+\varepsilon)\binom{\varepsilon}{\varepsilon/2}} = \sum_{n=0}^{\infty} \beta_n \varepsilon^n. \quad (9.27)$$

Note that β_k is easy to compute; indeed, appealing to (9.8), we find that β_n evaluates in terms of $\log 3$ and zeta values. The expansion of hypergeometric functions in terms of their parameters as in (9.25) is commonly referred to as *epsilon expansion*.

Let $S_k(j) := \sum_{m=1}^j \frac{1}{m^k}$ denote the harmonic numbers of order k . Following [83] we abbreviate $S_k := S_k(j-1)$. As in [82, Appendix B], we use the duplication

formula $(2a)_{2j} = 4^j (a)_j (a + 1/2)_j$ as well as the expansion

$$\frac{(m + a\varepsilon)_j}{(m)_j} = \exp \left[- \sum_{k=1}^{\infty} \frac{(-a\varepsilon)^k}{k} [S_k(j + m - 1) - S_k(m - 1)] \right] \quad (9.28)$$

for positive integer m , to write

$$\begin{aligned} {}_3F_2 \left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4} \right) &= \sum_{j=0}^{\infty} \frac{(1 + \varepsilon/2)_j^3}{4^j j!^2 (3/2 + \varepsilon/2)_j} = \sum_{j=0}^{\infty} \frac{(1 + \varepsilon/2)_j^4}{j!^2 (2 + \varepsilon)_{2j}} \\ &= \sum_{j=0}^{\infty} \frac{2}{j+1} \frac{1}{\binom{2(j+1)}{j+1}} \left[\frac{(1 + \varepsilon/2)_j}{j!} \right]^4 \left[\frac{(2 + \varepsilon)_{2j}}{(2j+1)!} \right]^{-1} \\ &= \sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} \exp \left[\sum_{k=1}^{\infty} \frac{(-\varepsilon)^k}{k} A_{k,j} \right], \end{aligned} \quad (9.29)$$

where

$$A_{k,j} := S_k(2j - 1) - 1 - 4 \frac{S_k(j - 1)}{2^k} = \sum_{m=2}^{2j-1} \frac{2(-1)^{m+1} - 1}{m^k}. \quad (9.30)$$

We can now read off the terms α_n of the ε -expansion (9.25):

Theorem 9.4. For $n = 0, 1, 2, \dots$

$$\alpha_n = [\varepsilon^n] {}_3F_2 \left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4} \right) = (-1)^n \sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} \sum \prod_{k=1}^n \frac{A_{k,j}^{m_k}}{m_k! k^{m_k}} \quad (9.31)$$

where the inner sum is over all non-negative integers m_1, \dots, m_n such that $m_1 + 2m_2 + \dots + nm_n = n$.

PROOF. Equation (9.31) may be derived from (9.29) using Faà di Bruno's formula for the n th derivative of the composition of two functions. \square

Example 9.4.1 (α_0, α_1 and α_2). In particular,

$$\alpha_1 = [\varepsilon] {}_3F_2 \left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4} \right) = - \sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} A_{1,j} = - \sum_{j=1}^{\infty} \frac{2}{j} \frac{1}{\binom{2j}{j}} [\bar{S}_1 - 2S_1 - 1]. \quad (9.32)$$

Such *multiple inverse binomial sums* are studied in [83]. Using [83, (2.20), (2.21)] we find

$$\alpha_0 = \frac{2\pi}{3\sqrt{3}}, \quad (9.33)$$

$$\alpha_1 = \frac{2}{3\sqrt{3}} \left[\pi - \pi \log 3 + \text{Ls}_2 \left(\frac{\pi}{3} \right) \right]. \quad (9.34)$$

For the term α_2 in the ε -expansion, (9.29) produces

$$\begin{aligned} [\varepsilon^2] {}_3F_2\left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4}\right) &= \sum_{j=1}^{\infty} \frac{1}{j} \frac{1}{\binom{2j}{j}} [A_{1,j}^2 + A_{2,j}] \\ &= \sum_{j=1}^{\infty} \frac{1}{j} \frac{1}{\binom{2j}{j}} [\bar{S}_2 - S_2 + (\bar{S}_1 - 2S_1)^2 - 2\bar{S}_1 + 4S_1]. \end{aligned}$$

Using [83, (2.8),(2.22)–(2.24)] we obtain

$$\begin{aligned} \alpha_2 &= \frac{2}{3\sqrt{3}} \left[\frac{\pi}{72} - \pi \log 3 + \frac{1}{2} \pi \log 3 + (1 - \log 3) \text{Ls}_2\left(\frac{\pi}{3}\right) \right. \\ &\quad \left. + \frac{3}{2} \text{Ls}_3\left(\frac{\pi}{3}\right) + \frac{3}{2} \text{Ls}_3\left(\frac{2\pi}{3}\right) - 3 \text{Ls}_3(\pi) \right]. \end{aligned} \quad (9.35)$$

◇

These results provide us with evaluations of $\mu_1(1+x+y)$ and $\mu_2(1+x+y)$.

Theorem 9.5 (Evaluation of $\mu_1(1+x+y)$ and $\mu_2(1+x+y)$). *We have*

$$\mu_1(1+x+y) = \frac{1}{\pi} \text{Ls}_2\left(\frac{\pi}{3}\right), \quad (9.36)$$

$$\mu_2(1+x+y) = \frac{3}{\pi} \text{Ls}_3\left(\frac{2\pi}{3}\right) + \frac{\pi^2}{4}. \quad (9.37)$$

PROOF. Using Theorem 9.3 we obtain

$$\mu_1(1+x+y) = \frac{3\sqrt{3}}{2\pi} [(\log 3 - 1)\alpha_0 + \alpha_1]. \quad (9.38)$$

Combining this with equations (9.33) and (9.34) yields (9.36). Again using Theorem 9.3 we find

$$\mu_2(1+x+y) = \frac{3\sqrt{3}}{2\pi} \left[(\log^2 3 - 2\log 3 + 2 - \frac{\pi^2}{12})\alpha_0 + 2(\log 3 - 1)\alpha_1 + 2\alpha_2 \right],$$

which, together with equations (9.33), (9.34) and (9.35), gives

$$\begin{aligned} \pi \mu_2(1+x+y) &= 3 \text{Ls}_3\left(\frac{2\pi}{3}\right) + 3 \text{Ls}_3\left(\frac{\pi}{3}\right) - 6 \text{Ls}_3(\pi) - \frac{\pi^3}{18} \\ &= 3 \text{Ls}_3\left(\frac{2\pi}{3}\right) + \frac{\pi^3}{4}. \end{aligned} \quad (9.39)$$

The last equality follows, for instance, automatically from the results in [54]. □

The evaluation of α_3 is more involved and we omit some details. Again, (9.29) produces

$$[\varepsilon^3] {}_3F_2\left(\begin{matrix} \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2}, \frac{\varepsilon+2}{2} \\ 1, \frac{\varepsilon+3}{2} \end{matrix} \middle| \frac{1}{4}\right) = -\frac{1}{3} \sum_{j=1}^{\infty} \frac{1}{j} \frac{1}{\binom{2j}{j}} [A_{1,j}^3 + 3A_{1,j}A_{2,j} + 2A_{3,j}].$$

Using [83, (2.25)–(2.28), (2.68)–(2.70), (2.81), (2.89)] as well as results from [54] we are led to

$$\begin{aligned} \alpha_3 = & \frac{2}{3\sqrt{3}} \left[\frac{5\pi^3}{108} (1 - \log 3) + \frac{1}{2} \pi \log^2 3 - \frac{1}{6} \pi \log^3 3 + \frac{11}{9} \pi \zeta(3) \right. \\ & + \text{Cl}_2 \left(\frac{\pi}{3} \right) \left(\frac{5}{36} \pi^2 - \log 3 + \frac{1}{2} \log^2 3 \right) - 3 \text{Gl}_{2,1} \left(\frac{2\pi}{3} \right) (1 - \log 3) \\ & \left. - \frac{35}{6} \text{Cl}_4 \left(\frac{\pi}{3} \right) + 15 \text{Cl}_{2,1,1} \left(\frac{2\pi}{3} \right) - 3 \text{Lsc}_{2,3} \left(\frac{\pi}{3} \right) \right]. \end{aligned} \quad (9.40)$$

Observe the occurrence of $\text{Lsc}_{2,3} \left(\frac{\pi}{3} \right)$ defined in (9.12). Proceeding as in the proof of Theorem 9.5 we obtain:

Theorem 9.6 (Evaluation of $\mu_3(1+x+y)$). *We have*

$$\begin{aligned} \pi \mu_3(1+x+y) = & 15 \text{Ls}_4 \left(\frac{2\pi}{3} \right) - 18 \text{Lsc}_{2,3} \left(\frac{\pi}{3} \right) - 15 \text{Cl}_4 \left(\frac{\pi}{3} \right) \\ & - \frac{1}{4} \pi^2 \text{Cl}_2 \left(\frac{\pi}{3} \right) - 17 \pi \zeta(3). \end{aligned} \quad (9.41)$$

The log-sine-cosine integral appears to reduce further as

$$12 \text{Lsc}_{2,3} \left(\frac{\pi}{3} \right) \stackrel{?}{=} 6 \text{Ls}_4 \left(\frac{2\pi}{3} \right) - 4 \text{Cl}_4 \left(\frac{\pi}{3} \right) - 7 \pi \zeta(3). \quad (9.42)$$

This conjectural reduction also appears in [82, (A.30)] where it was found via PSLQ. Combining with (9.41), we obtain an conjectural evaluation of $\mu_3(1+x+y)$ equivalent to (9.82).

9.5. Trigonometric analysis of $\mu_n(1+x+y)$

In light of (9.24) we define

$$\rho_n(\alpha) := \frac{1}{2\pi} \int_{-\pi}^{\pi} (\text{Re} \log(1 - \alpha e^{i\omega}))^n d\omega \quad (9.43)$$

for $n \geq 0$, so that

$$\mu_n(1+x+y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \rho_n(|2 \sin \theta|) d\theta. \quad (9.44)$$

In a sequence of combinatorial propositions, we study the properties of ρ_n .

Proposition 9.2 (Properties of ρ_n). *Let n be a positive integer.*

(a) *For $|\alpha| \leq 1$ we have*

$$\rho_n(\alpha) = (-1)^n \sum_{m=1}^{\infty} \frac{\alpha^m}{m^n} \omega_n(m), \quad (9.45)$$

where ω_n is defined as

$$\omega_n(m) = \sum_{\sum_{j=1}^n k_j = m} \frac{1}{2\pi} \int_{-\pi}^{\pi} \prod_{j=1}^n \frac{m}{k_j} \cos(k_j \omega) \, d\omega. \quad (9.46)$$

(b) For $|\alpha| \geq 1$ we have

$$\rho_n(\alpha) = \sum_{k=0}^n \binom{n}{k} \log^{n-k} |\alpha| \rho_k \left(\frac{1}{\alpha} \right). \quad (9.47)$$

PROOF. For (a) we use (9.43) to write

$$\begin{aligned} \rho_n(\alpha) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} (\operatorname{Re} \log(1 - \alpha e^{i\omega}))^n \, d\omega = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ -\sum_{k \geq 1} \frac{\alpha^k}{k} \cos(k\omega) \right\}^n \, d\omega \\ &= (-1)^n \sum_{m=1}^{\infty} \frac{\alpha^m}{m^n} \omega_n(m), \end{aligned}$$

as asserted. We note that $|\omega_n(m)| \leq m^n$ and so the sum is convergent.

For (b) we use (9.43) to write $\rho_n(\alpha) =$

$$\begin{aligned} &\frac{1}{2\pi} \int_{-\pi}^{\pi} \log^n (|\alpha| |1 - \alpha^{-1} e^{i\omega}|) \, d\omega = \frac{1}{2\pi} \int_{-\pi}^{\pi} (\log |\alpha| + \log |1 - \alpha^{-1} e^{i\omega}|)^n \, d\omega \\ &= \sum_{k=0}^n \binom{n}{k} \log^{n-k} |\alpha| \frac{1}{2\pi} \int_{-\pi}^{\pi} \log^k |1 - \alpha^{-1} e^{i\omega}| \, d\omega = \sum_{k=0}^n \binom{n}{k} \log^{n-k} |\alpha| \rho_k \left(\frac{1}{\alpha} \right), \end{aligned}$$

as required. \square

Example 9.5.1 (Evaluation of ω_n and ρ_n for $n \leq 2$). We have $\omega_0(m) = 0$, $\omega_1(m) = \delta_0(m)$, and

$$\omega_2(0) = 1, \quad \omega_2(2m) = 2, \quad \omega_2(2m+1) = 0. \quad (9.48)$$

Likewise, $\rho_0(\alpha) = 1$, $\rho_1(\alpha) = \log \max(|\alpha|, 1)$, and

$$\rho_2(\alpha) = \begin{cases} \frac{1}{2} \operatorname{Li}_2(\alpha^2) & \text{for } |\alpha| \leq 1, \\ \frac{1}{2} \operatorname{Li}_2\left(\frac{1}{\alpha^2}\right) + \log^2 |\alpha| & \text{for } |\alpha| \geq 1, \end{cases} \quad (9.49)$$

where the latter follows from (9.48) and Proposition 9.2. \diamond

We have arrived at the following description of $\mu_n(1+x+y)$:

Proposition 9.3 (Evaluation of $\mu_n(1+x+y)$). *Let n be a positive integer. Then*

$$\begin{aligned} \mu_n(1+x+y) &= \frac{1}{\pi} \left\{ \operatorname{Ls}_{n+1} \left(\frac{\pi}{3} \right) - \operatorname{Ls}_{n+1}(\pi) \right\} + \frac{2}{\pi} \int_0^{\pi/6} \rho_n(2 \sin \theta) \, d\theta \\ &\quad + \frac{2}{\pi} \sum_{k=2}^n \binom{n}{k} \int_{\pi/6}^{\pi/2} \log^{n-k}(2 \sin \theta) \rho_k \left(\frac{1}{2 \sin \theta} \right) \, d\theta. \end{aligned} \quad (9.50)$$

PROOF. Since $|\alpha| < 1$ when $|\theta| < \pi/6$, we start with (9.44) to get

$$\begin{aligned} \mu_n(1+x+y) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \rho_n(|2\sin\theta|) d\theta \\ &= \frac{2}{\pi} \int_0^{\pi/6} \rho_n(2\sin\theta) d\theta + \frac{2}{\pi} \int_{\pi/6}^{\pi/2} \rho_n(2\sin\theta) d\theta \\ &= \frac{2}{\pi} \int_0^{\pi/6} \rho_n(2\sin\theta) d\theta + \sum_{k=0}^n \binom{n}{k} \frac{2}{\pi} \int_{\pi/6}^{\pi/2} \log^{n-k}(2\sin\theta) \rho_k\left(\frac{1}{2\sin\theta}\right) d\theta. \end{aligned}$$

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 (9.50). □

As can be easily shown, we have the following multiple Mahler measure,

$$\pi \mu(1+x+y_1, 1+x+y_2, \dots, 1+x+y_n) = \text{Ls}_{n+1}\left(\frac{\pi}{3}\right) - \text{Ls}_{n+1}(\pi). \tag{9.51}$$

We record the following for log-sine values at $\pi/3$:

Example 9.5.2 (Values of $\text{Ls}_n(\pi/3)$). The following evaluations hold [54]:

$$\begin{aligned} \text{Ls}_2\left(\frac{\pi}{3}\right) &= \text{Cl}_2\left(\frac{\pi}{3}\right) \\ -\text{Ls}_3\left(\frac{\pi}{3}\right) &= \frac{7}{108} \pi^3 \\ \text{Ls}_4\left(\frac{\pi}{3}\right) &= \frac{1}{2} \pi \zeta(3) + \frac{9}{2} \text{Cl}_4\left(\frac{\pi}{3}\right) \\ -\text{Ls}_5\left(\frac{\pi}{3}\right) &= \frac{1543}{19440} \pi^5 - 6 \text{Gl}_{4,1}\left(\frac{\pi}{3}\right) \\ \text{Ls}_6\left(\frac{\pi}{3}\right) &= \frac{15}{2} \pi \zeta(5) + \frac{35}{36} \pi^3 \zeta(3) + \frac{135}{2} \text{Cl}_6\left(\frac{\pi}{3}\right). \end{aligned}$$

These evaluations use the method from [95]. On the other hand, $\text{Ls}_n^{(1)}(\pi/3)$ also lends itself nicely to analysis. From the integral definition (9.6), we make a change of variable $x = 2\sin(\theta/2)$, expand the new integrand as a series, integrate by parts then finally interchange the order of integration and summation. The result is

$$\text{Ls}_n^{(1)}\left(\frac{\pi}{3}\right) = \frac{-(n-2)!}{(-2)^{n-2}} \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k} k^n}. \tag{9.52}$$

With the right hand sum, we use the standard trick and identify the *inverse binomial* coefficient as its beta integral, $n \int_0^1 t^{n-1}(1-t)^n dt$. Interchanging the order of summation and integration once more, we have

$$\text{Ls}_n^{(1)}\left(\frac{\pi}{3}\right) = \frac{-(n-2)!}{(-2)^{n-2}} \int_0^1 \text{Li}_{n-1}(t(1-t)) \frac{dt}{t}. \tag{9.53}$$

Equations (9.52) and (9.53) then give a number of evaluations, such as

$$\text{Ls}_3^{(1)}\left(\frac{\pi}{3}\right) = \frac{\pi}{3}\text{Cl}_2\left(\frac{\pi}{3}\right) - \frac{2\zeta(3)}{3},$$

while an evaluation for $\text{Ls}_4^{(1)}(\pi/3)$ gives the hypergeometric identity

$${}_5F_4\left(\begin{matrix} 1, 1, 1, 1, 1 \\ \frac{3}{2}, 2, 2, 2 \end{matrix} \middle| \frac{1}{4}\right) = \frac{17}{18}\zeta(4),$$

compare with the hypergeometric form coming from $\text{Ls}_n(\pi/3)$ via (9.10), e. g.

$${}_4F_3\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ \frac{3}{2}, \frac{3}{2}, \frac{3}{2} \end{matrix} \middle| \frac{1}{4}\right) = \frac{7\pi^3}{216}.$$

◇

9.5.1. Further evaluation of ρ_n . To make further progress, we need first to determine ρ_n for $n \geq 3$. It is instructive to explore the next few cases.

Example 9.5.3 (Evaluation of ω_3 and ρ_3). We use the trigonometric identity

$$4 \cos(a) \cos(b) \cos(c) = \cos(a+b+c) + \cos(a-b-c) + \cos(a-b+c) + \cos(a-c+b)$$

to derive

$$\omega_3(m) = \frac{1}{4} \sum \left\{ \frac{m^3}{ijk} : i \pm j \pm k = 0, i + j + k = m \right\}.$$

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,

$$\omega_3(2m) = \frac{3}{4} \sum_{j+k=m} \frac{(2m)^3}{jk(j+k)} = 6 \sum_{j+k=m} \frac{m^2}{jk} = 12m \sum_{k=1}^{m-1} \frac{1}{k}. \quad (9.54)$$

Hence, by Proposition 9.2,

$$\rho_3(\alpha) = -\frac{3}{2} \sum_{m=1}^{\infty} \frac{\sum_{k=1}^{m-1} \frac{1}{k}}{m^2} \alpha^{2m} = -\frac{3}{2} \text{Li}_{2,1}(\alpha^2) \quad (9.55)$$

for $|\alpha| < 1$.

◇

In the general case we have

$$\prod_{j=1}^n \cos(x_j) = 2^{-n} \sum_{\varepsilon \in \{-1,1\}^n} \cos\left(\sum_{j=1}^n \varepsilon_j x_j\right) \quad (9.56)$$

which follows inductively from $2 \cos(a) \cos(b) = \cos(a+b) + \cos(a-b)$.

Proposition 9.4. For integers $n, m \geq 0$ we have $\omega_n(2m + 1) = 0$.

PROOF. In light of (9.56), the summand corresponding to the indices k_1, \dots, k_n in (9.46) for $\omega_n(2m+1)$ is nonzero if and only if there exists $\varepsilon \in \{-1, 1\}^n$ such that $\varepsilon_1 k_1 + \dots + \varepsilon_n k_n = 0$. In other words, there is a set $S \subset \{1, \dots, n\}$ such that

$$\sum_{j \in S} k_j = \sum_{j \notin S} k_j.$$

Thus $k_1 + \dots + k_n = 2 \sum_{j \in S} k_j$ which contradicts $k_1 + \dots + k_n = 2m + 1$. \square

Example 9.5.4 (Evaluation of ω_4 and ρ_4). Proceeding as in Example 9.5.3 and employing (9.56), we find

$$\begin{aligned} \omega_4(2m) &= \frac{3}{8} \sum_{\substack{i+j=m \\ k+l=m}} \frac{(2m)^4}{ijkl} + \frac{1}{2} \sum_{i+j+k=m} \frac{(2m)^4}{ijk\ell} = 24m^2 \sum_{\substack{i < m \\ j < m}} \frac{1}{ij} + 24m^2 \sum_{i+j < m} \frac{1}{ij} \\ &= 48m^2 \sum_{i=1}^{m-1} \frac{1}{i} \sum_{j=1}^{i-1} \frac{1}{j} + 24m^2 \sum_{i=1}^{m-1} \frac{1}{i^2} + 48m^2 \sum_{i=1}^{m-1} \frac{1}{i} \sum_{j=1}^{i-1} \frac{1}{j}. \end{aligned} \quad (9.57)$$

Consequently, for $|\alpha| < 1$ and appealing to Proposition 9.2,

$$\rho_4(\alpha) = \sum_{m=1}^{\infty} \frac{\alpha^{2m}}{(2m)^4} \omega_4(2m) = 6 \operatorname{Li}_{2,1,1}(\alpha^2) + \frac{3}{2} \operatorname{Li}_{2,2}(\alpha^2). \quad (9.58)$$

This suggests that $\rho_n(\alpha)$ is generally expressible as a sum of polylogarithmic terms, as will be shown next. \diamond

For the general evaluation of $\omega_n(2m)$, for integers $j \geq 0$ and $m \geq 1$, define

$$\sigma_j(m) := \sum_{m_1 + \dots + m_j = m} \frac{1}{m_1 \cdots m_j}. \quad (9.59)$$

Proposition 9.5. For positive integers n, m we have

$$\frac{\omega_n(2m)}{m^n} = \sum_{j=1}^{n-1} \binom{n}{j} \sigma_j(m) \sigma_{n-j}(m) \quad (9.60)$$

where σ_j is defined in (9.59).

PROOF. It follows from (9.56) that

$$\omega_n(2m) = \sum_{k_1 + \dots + k_n = 2m} \sum_{\sum_j \varepsilon_j k_j = 0} \prod_{j=1}^n \frac{m}{k_j}.$$

Arguing as in Proposition 9.4 we therefore find that

$$\omega_n(2m) = \sum_{j=1}^{n-1} \binom{n}{j} \sum_{\substack{k_1 + \dots + k_j = m \\ k_{j+1} + \dots + k_n = m}} \prod_{j=1}^n \frac{m}{k_j}.$$

This is equivalent to (9.60). □

Moreover, we obtain a simple recursion:

Proposition 9.6. *Let $m \geq 1$. Then $\sigma_1(m) = 1/m$ while for $j \geq 2$ we have*

$$\sigma_j(m) = \frac{j}{m} \sum_{r=1}^{m-1} \sigma_{j-1}(r), \tag{9.61}$$

$$= \frac{j!}{m} \sum_{m > m_1 > \dots > m_{j-1} > 0} \frac{1}{m_1 \cdots m_{j-1}}. \tag{9.62}$$

PROOF. This follows by simple combinatorics. We have

$$\begin{aligned} \sigma_j(m) &= \sum_{m_1 + \dots + m_j = m} \frac{1}{m_1 \cdots m_j} = \frac{1}{m} \sum_{m_1 + \dots + m_j = m} \frac{m_1 + \dots + m_j}{m_1 \cdots m_j} \\ &= \frac{j}{m} \sum_{m_1 + \dots + m_j = m} \frac{1}{m_1 \cdots m_{j-1}} = \frac{j}{m} \sum_{r=1}^{m-1} \sum_{m_1 + \dots + m_{j-1} = r} \frac{1}{m_1 \cdots m_{j-1}} \end{aligned}$$

which yields (9.61). Iterating (9.61) gives (9.62). □

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 9.5.3 and 9.5.4. To further illustrate Propositions 9.5 and 9.6, we now compute ρ_5 and ρ_6 .

Example 9.5.5 (Evaluation of ρ_5 and ρ_6). From Proposition 9.5,

$$\frac{\omega_5(2m)}{m^5} = 10\sigma_1(m)\sigma_4(m) + 20\sigma_2(m)\sigma_3(m).$$

Consequently, for $|\alpha| < 1$,

$$-\rho_5(\alpha) = \sum_{m=1}^{\infty} \frac{\alpha^{2m}}{(2m)^5} \omega_5(2m) = 30 \operatorname{Li}_{2,1,1,1,1}(\alpha^2) + \frac{15}{2} (\operatorname{Li}_{2,1,2}(\alpha^2) + \operatorname{Li}_{2,2,1}(\alpha^2)). \tag{9.63}$$

Similarly, $\rho_6(\alpha) =$

$$180 \operatorname{Li}_{2,1,1,1,1,1}(\alpha^2) + 45 (\operatorname{Li}_{2,1,1,2}(\alpha^2) + \operatorname{Li}_{2,1,2,1}(\alpha^2) + \operatorname{Li}_{2,2,1,1}(\alpha^2)) + \frac{45}{4} \operatorname{Li}_{2,2,2}(\alpha^2).$$

◇

In general, ρ_n evaluates as follows:

Proposition 9.7 (Evaluation of ρ_n). *For $|\alpha| < 1$ and integers $n \geq 2$,*

$$\rho_n(\alpha) = \frac{(-1)^n n!}{4^n} \sum_w 4^{\ell(w)} \operatorname{Li}_w(\alpha^2)$$

where the sum is over all indices $w = (2, a_2, a_3, \dots, a_{\ell(w)})$ such that $a_2, a_3, \dots \in \{1, 2\}$ and $|w| = n$.

PROOF. From Proposition 9.5 and (9.62) we have

$$\rho_n(\alpha) = \frac{(-1)^n n!}{2^n} \sum_{m=1}^{\infty} \frac{\alpha^{2m}}{m^2} \sum_{j=0}^{n-2} \sum_{\substack{m > m_1 > \dots > m_j > 0 \\ m > m_{j+1} > \dots > m_{n-2} > 0}} \frac{1}{m_1 \cdots m_{n-2}}.$$

Combining the right-hand side into polylogarithms yields

$$\rho_n(\alpha) = \frac{(-1)^n n!}{2^n} \sum_{k=0}^{n-2} \sum_{\substack{a_1, \dots, a_k \in \{1, 2\} \\ a_1 + \dots + a_k = n-2}} 2^{c(a)} \operatorname{Li}_{2, a_1, \dots, a_k}(\alpha^2)$$

where $c(a)$ is the number of 1's among a_1, \dots, a_k . The claim follows. \square

9.5.2. Reducing multiple polylogarithms of weight < 5 . Propositions 9.3 and 9.7 take us closer to a closed form for $\mu_n(1+x+y)$. As ρ_n are expressible in terms of multiple polylogarithms of weight n , it remains to supply reductions for those of low weight. Such polylogarithms are reduced [50] 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 greater than 1 or not (the operator D_i reduces the outer index of f by 1, or in the case that it is already 1, removes it altogether). Such operators give rise to the *shuffle* relations which are very important in analysing multiple zeta values (for instance, it is conjectured that all algebraic relations among multiple zeta values arise from shuffle and stuffle relations; see also Chapter 13).

As was known to Ramanujan, and studied in [48], that for $0 < x < 1$,

$$\operatorname{Li}_{2,1}(x) = \frac{1}{2} \log^2(1-x) \log(x) + \log(1-x) \operatorname{Li}_2(1-x) - \operatorname{Li}_3(1-x) + \zeta(3). \quad (9.64)$$

For $\operatorname{Li}_{1,3}(x)$, since $(1-x) \operatorname{Li}'_{1,3}(x) = \operatorname{Li}_3(x)$, we get

$$\operatorname{Li}_{1,3}(x) = -\frac{1}{2} \operatorname{Li}_2^2(x) - \log(1-x) \operatorname{Li}_3(x). \quad (9.65)$$

For $\operatorname{Li}_{2,2}$ we work as follows. As $(1-x) \operatorname{Li}'_{1,2}(x) = \operatorname{Li}_2(x)$, integration yields

$$\begin{aligned} \operatorname{Li}_{1,2}(x) &= 2 \operatorname{Li}_3(1-x) - \log(1-x) \operatorname{Li}_2(x) - 2 \log(1-x) \operatorname{Li}_2(1-x) \\ &\quad - \log^2(1-x) \log(x) - 2\zeta(3). \end{aligned} \quad (9.66)$$

Then, since $x \operatorname{Li}'_{2,2}(x) = \operatorname{Li}_{1,2}(x)$, we integrate again and appeal to various formulas in [134, §6.4.4] to arrive at

$$\begin{aligned} \operatorname{Li}_{2,2}(t) &= \frac{1}{2} \log^2(1-t) \log^2 t - 2\zeta(2) \log(1-t) \log t - 2\zeta(3) \log t - \frac{1}{2} \operatorname{Li}_2^2(t) \\ &\quad + 2 \operatorname{Li}_3(1-t) \log t - 2 \int_0^t \frac{\operatorname{Li}_2(x) \log x}{1-x} dx - \int_0^t \frac{\log(1-x) \log^2 x}{1-x} dx. \end{aligned}$$

Expanding the penultimate integral as a series leads to

$$\int_0^t \frac{\operatorname{Li}_2(x) \log x}{1-x} dx = \operatorname{Li}_{1,2}(t) \log t - \operatorname{Li}_{2,2}(t).$$

(Observe that fortunately for us, $\operatorname{Li}_{2,2}$ does not cancel out in this analysis.) Then, using [134, A3.4 Eqn. (12)] to evaluate the remaining integral, we deduce that

$$\begin{aligned} \operatorname{Li}_{2,2}(x) &= -\frac{1}{12} \log^4(1-x) + \frac{1}{3} \log^3(1-x) \log x - \zeta(2) \log^2(1-x) \\ &\quad + 2 \log(1-x) \operatorname{Li}_3(x) - 2\zeta(3) \log(1-x) - 2 \operatorname{Li}_4(x) \\ &\quad - 2 \operatorname{Li}_4\left(\frac{x}{x-1}\right) + 2 \operatorname{Li}_4(1-x) - 2\zeta(4) + \frac{1}{2} \operatorname{Li}_2^2(x). \end{aligned} \quad (9.67)$$

The form for $\operatorname{Li}_{3,1}(x)$ is obtained starting from $\operatorname{Li}_{2,1}(x)$. This gives:

$$2 \operatorname{Li}_{3,1}(x) + \operatorname{Li}_{2,2}(x) = \frac{1}{2} \operatorname{Li}_2^2(x). \quad (9.68)$$

This result, and its derivative

$$2 \operatorname{Li}_{2,1}(x) + \operatorname{Li}_{1,2}(x) = \operatorname{Li}_1(x) \operatorname{Li}_2(x),$$

are also obtained in [204, Cor. 2 & Cor. 3] by other methods.

Dividing the expression for $\operatorname{Li}_{1,2}(x)$ by $1-x$ and integrate, we obtain

$$\begin{aligned} \operatorname{Li}_{1,1,2}(x) &= \frac{\pi^4}{30} + \frac{\pi^2}{12} \log^2(1-x) + \log(1-x) \operatorname{Li}_3(1-x) \\ &\quad - 3 \operatorname{Li}_4(1-x) + 2\zeta(3) \log(1-x). \end{aligned}$$

Similarly,

$$\begin{aligned} \operatorname{Li}_{1,2,1}(x) &= -\frac{\pi^4}{30} + \frac{1}{2} \log^2(1-x) \operatorname{Li}_2(1-x) - 2 \log(1-x) \operatorname{Li}_3(1-x) \\ &\quad + 3 \operatorname{Li}_4(1-x) - \zeta(3) \log(1-x). \end{aligned}$$

Since $\text{Li}_{2,1,1}(x) = \int_0^x \text{Li}_{1,1,1}(t)/t dt$ and $\text{Li}_{1,1,1}(x) = \int_0^x \text{Li}_{1,1}(t)/(1-t) dt$, we first compute $\text{Li}_{1,1}(x) = \log^2(1-x)/2$ to find that $\text{Li}_{1,1,1}(x) = -\log^3(1-x)/6$. Hence

$$\begin{aligned} \text{Li}_{2,1,1}(x) &= -\frac{1}{6} \int_0^x \log^3(1-t) \frac{dt}{t} = \frac{\pi^4}{90} - \frac{1}{6} \log^2(1-x) \log x \\ &\quad - \frac{1}{2} \log^2(1-x) \text{Li}_2(1-x) + \log(1-x) \text{Li}_3(1-x) - \text{Li}_4(1-x). \end{aligned} \quad (9.69)$$

In general,

$$\text{Li}_{\{1\}^n}(x) = \frac{(-1)^n}{n!} \log(1-x)^n, \quad (9.70)$$

and therefore

$$\begin{aligned} \text{Li}_{2,\{1\}^{n-1}}(x) &= \frac{(-1)^n}{n!} \int_0^x \log(1-t)^n \frac{dt}{t} \\ &= \zeta(n+1) - \sum_{m=0}^n \frac{(-1)^{n-m}}{(n-m)!} \log(1-x)^{n-m} \text{Li}_{m+1}(1-x). \end{aligned} \quad (9.71)$$

We have, inter alia, provided closed reductions for *all* multiple polylogarithms of weight less than five. One does not expect such complete results thereafter.

Example 9.5.6 (Multiple zeta values). By taking the limit $x \rightarrow 1^-$ in (9.64), one recovers the celebrated result

$$\zeta(2, 1) = \zeta(3).$$

Similarly, (9.69) gives $\zeta(2, 1, 1) = \zeta(4)$, and with the help of [134, p. 301, (40)], we get $\zeta(2, 2) = \pi^4/120$ and $\zeta(3, 1) = \pi^4/360$. See also Chapter 13. \diamond

The reductions in this section allow us to express ρ_3 and ρ_4 in terms of polylogarithms of depth 1. Equation (9.64) treats ρ_3 while (9.58) leads to

$$\begin{aligned} \rho_4(\alpha^2) &= 3(\text{Li}_3(\alpha^2) - \zeta(3) + \text{Li}_3(1-\alpha^2)) \log(1-\alpha^2) - \frac{1}{8} \log^4(1-\alpha^2) \\ &\quad + 3\zeta(4) - 3 \text{Li}_4\left(\frac{-\alpha^2}{1-\alpha^2}\right) - 3 \text{Li}_4(\alpha^2) - 3 \text{Li}_4(1-\alpha^2) + \frac{3}{4} \text{Li}_2^2(1-\alpha^2) \\ &\quad - \log \alpha \log^3(1-\alpha^2) - \left(\frac{\pi^2}{4} + 3 \text{Li}_2(1-\alpha^2)\right) \log^2(1-\alpha^2). \end{aligned} \quad (9.72)$$

9.6. Evaluation of $\mu_2(1+x+y)$

We review the evaluation of $\mu_2(1+x+y)$ from [55], a result derived alternatively in Theorem 9.5.

Proposition 9.8 (A dilogarithmic representation). *We have*

$$(a) \quad \frac{1}{\pi} \int_0^\pi \operatorname{Re} \operatorname{Li}_2(4 \sin^2 \theta) \, d\theta = \zeta(2), \quad (9.73)$$

$$(b) \quad \mu_2(1+x+y) = \frac{\pi^2}{36} + \frac{2}{\pi} \int_0^{\pi/6} \operatorname{Li}_2(4 \sin^2 \theta) \, d\theta. \quad (9.74)$$

PROOF. For (a) we define the analytic function $\tau(z) := \frac{1}{\pi} \int_0^\pi \operatorname{Li}_2(4z \sin^2 \theta) \, d\theta$. For $|z| < 1/4$ we may use the defining series for Li_2 and expand term by term using Wallis' formula to derive

$$\begin{aligned} \tau(z) &= \frac{1}{\pi} \sum_{n \geq 1} \frac{(4z)^n}{n^2} \int_0^\pi \sin^{2n} \theta \, d\theta = 2z {}_4F_3 \left(\begin{matrix} 1, 1, 1, \frac{3}{2} \\ 2, 2, 2 \end{matrix} \middle| 4z \right) \\ &= 2 \operatorname{Li}_2 \left(\frac{1}{2} - \frac{1}{2} \sqrt{1-4z} \right) - \log \left(\frac{1}{2} + \frac{1}{2} \sqrt{1-4z} \right)^2. \end{aligned}$$

The final equality can be obtained in *Mathematica* and then proven by differentiation (such is one advantage of using experimental mathematics). In particular, the final function provides an analytic continuation from which we obtain $\tau(1) = \zeta(2) + 2i \operatorname{Cl}_2(\frac{\pi}{3})$. This yields the assertion. (Note the similarity between this proof and the proof of Theorem 1.6.)

For (b), commencing much as in [126, Thm. 11], we write

$$\mu_2(1+x+y) = \frac{1}{4\pi^2} \int_{-\pi}^\pi \int_{-\pi}^\pi \operatorname{Re} \log(1 - 2 \sin(\theta) e^{i\omega})^2 \, d\omega \, d\theta.$$

We consider the inner integral $\rho(\alpha) := \int_{-\pi}^\pi (\operatorname{Re} \log(1 - \alpha e^{i\omega}))^2 \, d\omega$ with $\alpha := 2 \sin \theta$. For $|\theta| \leq \pi/6$ we directly apply Parseval's formula to obtain

$$\rho(2 \sin \theta) = \pi \operatorname{Li}_2(4 \sin^2 \theta) \quad (9.75)$$

which is equivalent to (9.49). In the remaining case we write

$$\begin{aligned} \rho(\alpha) &= \int_{-\pi}^\pi \left[\log |\alpha| + \operatorname{Re} \log(1 - \alpha^{-1} e^{i\omega}) \right]^2 \, d\omega \\ &= 2\pi \log^2 |\alpha| - 2 \log |\alpha| \int_{-\pi}^\pi \log |1 - \alpha^{-1} e^{i\omega}| \, d\omega + \pi \operatorname{Li}_2 \left(\frac{1}{\alpha^2} \right) \\ &= 2\pi \log^2 |\alpha| + \pi \operatorname{Li}_2 \left(\frac{1}{\alpha^2} \right), \end{aligned} \quad (9.76)$$

where we have appealed to Parseval's and Jensen's formulas. Thus,

$$\mu_2(1+x+y) = \frac{1}{\pi} \int_0^{\pi/6} \operatorname{Li}_2(4 \sin^2 \theta) \, d\theta + \frac{1}{\pi} \int_{\pi/6}^{\pi/2} \operatorname{Li}_2 \left(\frac{1}{4 \sin^2 \theta} \right) \, d\theta + \frac{\pi^2}{54}, \quad (9.77)$$

since

$$\frac{2}{\pi} \int_{\pi/6}^{\pi/2} \log^2 \alpha \, d\theta = \mu(1+x+y_1, 1+x+y_2) = \frac{\pi^2}{54}$$

by (9.51). Now, for $\alpha > 1$, the functional equation [134, A2.1 (6)]

$$\operatorname{Li}_2(\alpha) + \operatorname{Li}_2(1/\alpha) + \frac{1}{2} \log^2 \alpha = 2\zeta(2) + i\pi \log \alpha \quad (9.78)$$

gives

$$\int_{\pi/6}^{\pi/2} \left[\operatorname{Re} \operatorname{Li}_2(4 \sin^2 \theta) + \operatorname{Li}_2\left(\frac{1}{4 \sin^2 \theta}\right) \right] d\theta = \frac{5}{54} \pi^3. \quad (9.79)$$

We then combine (9.73), (9.79) and (9.77) to deduce the desired result (9.74). \square

Remark 9.6.1 (Using ρ_2). The utility of the propositions in Section 9.5 can now be seen. Using the evaluation of ρ_2 and Proposition 9.3, we arrive at (9.77) immediately, from which it is a few short steps to equation (9.74).

Following [55], we expand out the Li_2 term in (9.74) as a series then interchange the order of integration and summation. This is equivalent to, after passing to a ${}_2F_1$,

$$\begin{aligned} \mu_2(1+x+y) &= \frac{\pi^2}{36} + \frac{\sqrt{3}}{\pi} \sum_{n=1}^{\infty} \frac{\binom{2n}{n}}{n^2} \int_0^{1/2} \frac{t^n(1-t)^n}{1-t+t^2} dt \\ &= \frac{\pi^2}{36} + \frac{\sqrt{3}}{\pi} \int_0^{1/2} \frac{2\operatorname{Li}_2(t) - \log^2(1-t)}{1-t+t^2} dt, \end{aligned}$$

where we have corrected a misprint in [55]. Simplifying the last integral using results in [134], we finally see (9.74) is equivalent to (9.37). \diamond

9.6.1. Conclusion. To recapitulate, $\mu_k(1+x+y) = W_3^{(k)}(0)$ has been evaluated in terms of log-sine integrals for $1 \leq k \leq 3$. Namely,

$$\mu_1(1+x+y) = \frac{3}{2\pi} \operatorname{Ls}_2\left(\frac{2\pi}{3}\right), \quad (9.80)$$

$$\mu_2(1+x+y) = \frac{3}{\pi} \operatorname{Ls}_3\left(\frac{2\pi}{3}\right) + \frac{\pi^2}{4}, \quad (9.81)$$

$$\mu_3(1+x+y) \stackrel{?}{=} \frac{6}{\pi} \operatorname{Ls}_4\left(\frac{2\pi}{3}\right) - \frac{9}{\pi} \operatorname{Cl}_4\left(\frac{\pi}{3}\right) - \frac{\pi}{4} \operatorname{Cl}_2\left(\frac{\pi}{3}\right) - \frac{13}{2} \zeta(3). \quad (9.82)$$

It is possible, though tiresome, to use Propositions 9.3 and 9.7 to give us a description for μ_3 which is close to (9.82); a less complete analysis for μ_4 is also possible. The details are given in [41]. However, at least by the route chosen there, the technicalities of formalising (9.82) appear to be difficult.

Legendre Polynomials and Ramanujan-type Series for $1/\pi$

ABSTRACT. We resolve a family of identities involving $1/\pi$ using the theory of modular forms and hypergeometric series. In particular, we resort to a formula of Brafman which relates a generating function of the Legendre polynomials to a product of two Gaussian hypergeometric functions. Using our methods, we also derive some new Ramanujan-type series.

10.1. Introduction

In 2011, Z.-W. Sun [183] and G. Almkvist experimentally observed several new identities for $1/\pi$ of the form

$$\sum_{n=0}^{\infty} \frac{(s)_n (1-s)_n}{n!^2} (A + Bn) T_n(b, c) \lambda^n = \frac{C}{\pi}, \quad (10.1)$$

where $s \in \{1/2, 1/3, 1/4\}$, $A, B, b, c \in \mathbb{Z}$, $T_n(b, c)$ denotes the coefficient of x^n in the expansion of $(x^2 + bx + c)^n$, viz.

$$T_n(b, c) = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{2k} \binom{2k}{k} b^{n-2k} c^k, \quad (10.2)$$

while λ and C are either rational or (linear combinations of) quadratic irrationalities. All such equalities from [183] are compactly listed in Table 1.

The binomial sums (10.2) can be expressed via the *Legendre polynomials*

$$P_n(x) = {}_2F_1 \left(\begin{matrix} -n, n+1 \\ 1 \end{matrix} \middle| \frac{1-x}{2} \right)$$

by means of the formula

$$T_n(b, c) = (b^2 - 4c)^{n/2} P_n \left(\frac{b}{(b^2 - 4c)^{1/2}} \right),$$

so that equalities (10.1) assume the form

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} (A + Bn) P_n(x_0) z_0^n = \frac{C}{\pi}. \quad (10.3)$$

Note that representation by T_n is not unique, since $T_n(b, c) = a^n T_n(b/a, c/a^2)$.

The sequence of Legendre polynomials can be alternatively defined by the ordinary generating function

$$(1 - 2xz + z^2)^{-1/2} = \sum_{n=0}^{\infty} P_n(x) z^n.$$

In the rest of the chapter, we will make heavy use of another generating function for the Legendre polynomials due to F. Brafman. This and our general approach are described in Section 10.2. In Sections 10.3 – 10.6, we will examine the conjectures for $s = 1/2, 1/3, 1/4$ respectively, and indicate new identities (10.50)–(10.57) for $s = 1/4$ and $1/6$. Then in Sections 10.7 and 10.8 we show that “companion series” involving derivatives of Legendre polynomials can be obtained, and some of them, as well as a few series examined in the previous sections, are expressible in terms of known constants.

Our main result is the following, which we prove in Section 10.2:

Theorem 10.1. *All the series for $1/\pi$ listed in Table 1 are true.*

10.2. Brafman’s formula and modular equations

In [63], Brafman proved the following elegant hypergeometric formula for a generating function of the Legendre polynomials.

Proposition 10.1 (Brafman’s formula [63]).

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} P_n(x) z^n = {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| \frac{1-\rho-z}{2}\right) \cdot {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| \frac{1-\rho+z}{2}\right), \quad (10.4)$$

where $\rho = \rho(x, z) := (1 - 2xz + z^2)^{1/2}$.

This result has a more general form involving Jacobi polynomials. In [193] (Chapter 11) we follow the lines of Brafman’s derivation to prove a new type of generating functions for the Legendre polynomials.

By introducing the compact notation for the involved hypergeometric function and its derivative,

$$F(t) = F(s, t) := {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| t\right), \quad G(t) = G(s, t) := t \frac{d}{dt} F(t), \quad (10.5)$$

and differentiating both sides of (10.4) with respect to z , we immediately deduce

Proposition 10.2.

$$\sum_{n=0}^{\infty} \frac{(s)_n (1-s)_n}{n!^2} P_n(x) z^n = F(t_-) F(t_+), \quad (10.6)$$

$$\sum_{n=0}^{\infty} \frac{(s)_n (1-s)_n}{n!^2} n P_n(x) z^n = \frac{z(x-z-\rho)}{\rho(1-\rho-z)} G(t_-) F(t_+) + \frac{z(x-z+\rho)}{\rho(1-\rho+z)} F(t_-) G(t_+), \quad (10.7)$$

where $t_{\pm} = t_{\pm}(x, z) := (1 - \rho \pm z)/2$.

Note the notational difference between $F(s, t)$ here and $K^s(k)$ in Chapter 5.

For $s \in \{1/2, 1/3, 1/4, 1/6\}$ (the denominator of s is the *signature*), the right-hand side of Brafman's formula represents the product of two *arithmetic* [210] hypergeometric series: the modular functions

$$\begin{aligned} t_4(\tau) &= \left(1 + \frac{1}{16} \left(\frac{\eta(\tau)}{\eta(4\tau)}\right)^8\right)^{-1}, & t_3(\tau) &= \left(1 + \frac{1}{27} \left(\frac{\eta(\tau)}{\eta(3\tau)}\right)^{12}\right)^{-1}, \\ t_2(\tau) &= \left(1 + \frac{1}{64} \left(\frac{\eta(\tau)}{\eta(2\tau)}\right)^{24}\right)^{-1}, & t_1(\tau) &= \frac{1}{2} - \frac{1}{2} \sqrt{1 - \frac{1728}{j(\tau)}} \end{aligned} \quad (10.8)$$

(with subscripts denoting the *levels*) translate the respective series $F(t)$ into a weight 1 modular form $F(t(\tau))$. Here $\eta(\tau)$ and $j(\tau)$ are Dedekind's eta function and the modular invariant, respectively. For the rest of the chapter we will omit the subscript in $t_{\ell}(\tau)$ when the modular function used is clear from the context. The inversion formula is given [17, p. 91] by

$$\tau = iC_s \frac{F(1-t)}{F(t)}, \quad \text{where } C_s = \frac{1}{2 \sin \pi s} = \begin{cases} \frac{1}{2} & \text{if } s = \frac{1}{2}, \\ \frac{1}{\sqrt{3}} & \text{if } s = \frac{1}{3}, \\ \frac{1}{\sqrt{2}} & \text{if } s = \frac{1}{4}, \\ 1 & \text{if } s = \frac{1}{6}. \end{cases} \quad (10.9)$$

The elliptic nome is defined throughout the chapter as $q = e^{2\pi i\tau}$. Note that for any of the four modular functions in (10.8) we have

$$\frac{1}{2\pi i} \frac{dt}{d\tau} = q \frac{dt}{dq} = t(1-t)F^2(t), \quad (10.10)$$

the result already known to Ramanujan ([17, Chap. 33], [34], [80]).

When τ is a quadratic irrationality (with $\text{Im } \tau > 0$), the value $t(\tau)$ is known to be an algebraic number; computation of such values is well discussed in the literature – see, for example, [17, Chap. 34]. A common feature of the Sun–Almkvist series (10.3) from [183] for $s \in \{1/2, 1/3, 1/4\}$ is that the algebraic numbers

$$\alpha = \frac{1 - \rho_0 - z_0}{2} \quad \text{and} \quad \beta = \frac{1 - \rho_0 + z_0}{2}, \quad \text{where} \quad \rho_0 := (1 - 2x_0z_0 + z_0^2)^{1/2}, \quad (10.11)$$

are always values of the modular function $t(\tau)$ at two quadratic irrational points. In cases when x_0 and z_0 are *real*, we get $\alpha = t(\tau_0)$ and $\beta = t(\tau_0/N)$; while in cases when both x_0 and z_0 are *purely imaginary* (and there are five such cases in Table 1 marked by asterisk), we have $\alpha = t(\tau_0)$ and $\beta = 1 - t(\tau_0/N)$. The corresponding choice of quadratic irrationality τ_0 and integer $N > 1$ is given in Table 1. We also note that $|\alpha| \leq |\beta|$ for all entries, with strict inequality when both x_0 and z_0 are real.

Remark 10.2.1. Observe the duality between several entries in Table 1, where the roles of z_0 and ρ_0 are swapped. These correspond to the same choice of τ_0 with different choices of N , which is often a prime factor of an integer inside the radical in τ_0 . \diamond

Proposition 10.3. *In the notation of (10.11), assume that both α and β are within the convergence domain of the hypergeometric function $F(t)$ (that is, $|\alpha|, |\beta| < 1$).*

(a) *Suppose that $\alpha = t(\tau_0)$ and $\beta = t(\tau_0/N)$ for a quadratic irrational τ_0 and an integer $N > 1$. Then there exist effectively computable algebraic numbers μ_0 , λ_0 and λ_1 such that*

$$F(\beta) = \mu_0 F(\alpha) \quad \text{and} \quad G(\beta) = \lambda_0 F(\alpha) + \lambda_1 G(\alpha). \quad (10.12)$$

(b) *Suppose that $\alpha = t(\tau_0)$ and $\beta = 1 - t(\tau_0/N)$ for a quadratic irrational τ_0 and an integer $N > 1$. In addition, assume that $|1 - \beta| < 1$. Then there exist effectively*

computable algebraic numbers μ_0 , λ_0 , λ_1 and λ_2 such that

$$F(\beta) = \mu_0 F(\alpha) \quad \text{and} \quad G(\beta) = \lambda_0 F(\alpha) + \lambda_1 G(\alpha) + \frac{\lambda_2}{\pi F(\alpha)}. \quad (10.13)$$

PROOF. (a) For N given, the two modular functions $t(\tau)$ and $t(\tau/N)$ are related by the modular equation of degree N ; in particular, the function $t(\tau/N)$ is an algebraic function of $t(\tau)$. As both $F(t(\tau))$ and $F(t(\tau/N))$ are weight 1 modular forms, their quotient $F(t(\tau/N))/F(t(\tau))$ is a modular function, hence it is an algebraic function of $t(\tau)$. The quotient specialised at $\tau = \tau_0$ is then an algebraic number, which we denote by μ_0 .

Differentiating $F(t(\tau/N))/F(t(\tau))$ logarithmically and multiplying the result by $F^2(t(\tau))$, we arrive at a relation expressing $G(t(\tau/N))$ linearly via $F(t(\tau))$ and $G(t(\tau))$ with coefficients which are modular functions. Specialising at $\tau = \tau_0$ this yields the second equality in (10.12) with algebraic λ_0 and λ_1 .

(b) Consider now $\beta = 1 - \beta'$ where $\beta' = t(\tau_0/N)$. By what is shown in part (a),

$$F(\beta') = \mu'_0 F(\alpha) \quad \text{and} \quad G(\beta') = \lambda'_0 F(\alpha) + \lambda'_1 G(\alpha) \quad (10.14)$$

for certain algebraic μ'_0 , λ'_0 and λ'_1 . Relation (10.9) implies that

$$\frac{F(1-t)}{F(t)} = -\frac{i\tau}{C_s}, \quad (10.15)$$

which specialised to $\tau = \tau_0/N$, hence $t = \beta'$, results in

$$F(\beta) = -\frac{i\tau_0}{NC_s} F(\beta'). \quad (10.16)$$

Computing the logarithmic t -derivative of (10.15) and using (10.5), we find

$$\frac{tG(1-t)}{F(1-t)} + \frac{(1-t)G(t)}{F(t)} = -\frac{t(1-t)}{\tau} \left(\frac{dt}{d\tau}\right)^{-1} = \frac{it(1-t)F(t)}{C_s F(1-t)} \left(\frac{dt}{d\tau}\right)^{-1},$$

which, after multiplication by $F(1-t)/t$ and using (10.15), can be written as

$$G(1-t) = \frac{i\tau(1-t)}{C_s t} G(t) + \frac{i(1-t)}{C_s} F(t) \left(\frac{dt}{d\tau}\right)^{-1}. \quad (10.17)$$

Using now (10.10) and taking $\tau = \tau_0/N$ (so that $t = t(\tau_0/N) = \beta'$) in (10.17) we obtain

$$G(\beta) = \frac{i\tau_0\beta}{NC_s(1-\beta)} G(\beta') + \frac{1}{2\pi C_s(1-\beta)F(\beta')}. \quad (10.18)$$

Combining now (10.14), (10.16) and (10.18), we arrive at (10.13).

Finally note that all the above algebraicity is effectively computed by means of the involved modular equations. \square

Now we appeal to a particular case of Clausen's formula (1828) [11],

$${}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| t\right)^2 = {}_3F_2\left(\begin{matrix} \frac{1}{2}, s, 1-s \\ 1, 1 \end{matrix} \middle| 4t(1-t)\right), \quad (10.19)$$

which is valid for t within the left half of the lemniscate $4|t(1-t)| = 1$. Differentiating (10.19) and expanding the ${}_3F_2$ hypergeometric function into series, we obtain

Proposition 10.4. *For t satisfying $|t(1-t)| \leq 1/4$ and $\operatorname{Re} t < 1/2$,*

$$F^2(t) = \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (s)_n (1-s)_n}{n!^3} \cdot (4t(1-t))^n,$$

$$F(t)G(t) = \frac{1-2t}{2(1-t)} \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (s)_n (1-s)_n}{n!^3} \cdot n(4t(1-t))^n.$$

Our final argument goes back to Ramanujan's discovery [164] of hypergeometric formulas for $1/\pi$. Its proof is outlined in [35], [36], [46] and [77].

Proposition 10.5. *Let α be the value of the modular function $t(\tau)$ at a quadratic irrationality τ_0 . Assume that $|\alpha(1-\alpha)| \leq 1/4$ and $\operatorname{Re} \alpha < 1/2$. Then there exist effectively computable algebraic constants a, b and c such that*

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (s)_n (1-s)_n}{n!^3} (a+bn)(4\alpha(1-\alpha))^n = \frac{c}{\pi}. \quad (10.20)$$

Remark 10.2.2. Observe that all the values $\alpha = (1 - \rho_0 - z_0)/2$ from Table 1 satisfy the hypothesis of Proposition 10.5, with the exception of (III1) which we treat separately in Section 10.4. \diamond

PROOF OF THEOREM 10.1. For a given entry from Table 1, we choose $\alpha = (1 - \rho_0 - z_0)/2 = t(\tau_0)$ and $\beta = (1 - \rho_0 + z_0)/2$. Proposition 10.5 implies that we have a Ramanujan series (10.20). On invoking Proposition 10.4 for $t = \alpha$ we can write (10.20) in the form

$$aF^2(\alpha) + 2b\frac{1-\alpha}{1-2\alpha}F(\alpha)G(\alpha) = \frac{c}{\pi}. \quad (10.21)$$

On the other hand, by specialising the identities in Proposition 10.2 at $x = x_0$, $z = z_0$ and using then the algebraic relations obtained in Proposition 10.3 we obtain

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} P_n(x_0)z_0^n = \mu_0 F^2(\alpha),$$

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} n P_n(x_0)z_0^n = \lambda'_0 F^2(\alpha) + \lambda'_1 F(\alpha)G(\alpha) + \frac{\lambda'_2}{\pi},$$

with some algebraic (effectively computable) coefficients μ_0 , λ'_0 , λ'_1 and λ'_2 , where we simply choose $\lambda'_2 = 0$ if $\beta = t(\tau_0/N)$.

Finally, taking

$$B' = \frac{2b(1-\alpha)}{\lambda'_1(1-2\alpha)} \quad \text{and} \quad A' = \frac{a - B'\lambda'_0}{\mu_0}$$

we derive from (10.21) that

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} (A' + B'n) P_n(x_0)z_0^n = \frac{c - B'\lambda'_2}{\pi},$$

which assumes the required form (10.3) after setting $A = CA'/(c - B'\lambda'_2)$, $B = CB'/(c - B'\lambda'_2)$. \square

As verification of each entry in Table 1 requires an explicit knowledge of all the algebraic numbers involved and is therefore tedious, we give details for only some of the entries. In Section 10.3 we discuss in detail identity (I2) by using a parametrisation of the corresponding modular equation. Section 10.4 describes the techniques without using an explicit parametrisation on an example of identity (II1), and uses a hypergeometric transformation to treat (III1), an entry that does not satisfy the conditions of Proposition 10.5. Section 10.5 explains the derivation of identity (III5), which corresponds to imaginary x_0 and z_0 , as well as outlines new identities for $s = 1/4$. In Section 10.6 we present two identities corresponding to $s = 1/6$, which are not from the list in [183].

10.3. Identities for $s = 1/2$

We illustrate our techniques outlined in Section 10.2 with (I2),

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{n!^2} (7 + 30n) P_n\left(\frac{17}{12\sqrt{2}}\right) \left(-\frac{3}{4\sqrt{2}}\right)^n = \frac{12}{\pi}.$$

Here we have $N = 3$, so that the values $\alpha = t(\tau_0) = (1 - \rho_0 - z_0)/2$ and $\beta = t(\tau_0/3) = (1 - \rho_0 + z_0)/2$ are related by the modular polynomial [16, Chap. 19]

$$(\alpha^2 + \beta^2 + 6\alpha\beta)^2 - 16\alpha\beta(4(1 + \alpha\beta) - 3(\alpha + \beta))^2 = 0$$

and admit the rational parametrisation

$$\alpha = \frac{4\sqrt{2} - 5\sqrt{3} + 3}{8\sqrt{2}} = \frac{p^3(2+p)}{1+2p}, \quad p = \frac{3 - \sqrt{2} - \sqrt{3}}{2\sqrt{2}},$$

$$\beta = \frac{4\sqrt{2} - 5\sqrt{3} - 3}{8\sqrt{2}} = \frac{p(2+p)^3}{(1+2p)^3},$$

In the notation of (10.5), recall the identity [16, p. 238, Entry 6 (i)]

$$F\left(\frac{p(2+p)^3}{(1+2p)^3}\right) = (1+2p)F\left(\frac{p^3(2+p)}{1+2p}\right) \quad \text{for } p \in \left(-\frac{1}{2}, 1\right); \quad (10.22)$$

differentiating it we obtain

$$G\left(\frac{p(2+p)^3}{(1+2p)^3}\right) = \frac{p(1+2p)(2+p)}{(1-p)^2} F\left(\frac{p^3(2+p)}{1+2p}\right) + \frac{3(1+p)^2(1+2p)}{(1-p)^2} G\left(\frac{p^3(2+p)}{1+2p}\right). \quad (10.23)$$

Substituting $p = (3 - \sqrt{2} - \sqrt{3})/(2\sqrt{2})$ into (10.22) and (10.23) we obtain

$$F(\beta) = \frac{-\sqrt{6} + 3\sqrt{2}}{2} F(\alpha),$$

$$G(\beta) = -\frac{85\sqrt{6} + 120\sqrt{3} - 147\sqrt{2} - 208}{2} F(\alpha) + \frac{(-19\sqrt{3} + 33)(17\sqrt{2} + 24)}{2} G(\alpha).$$

Specialising (10.6), (10.7) by taking $x = 17/(12\sqrt{2})$, $z = -3/(4\sqrt{2})$ we get

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} (A + Bn) P_n\left(\frac{17}{12\sqrt{2}}\right) \left(\frac{-3}{4\sqrt{2}}\right)^n = \sqrt{6} \left(\frac{\sqrt{3}-1}{2} A - \frac{B}{30}\right) F^2(\alpha)$$

$$+ \frac{15\sqrt{2} + 8\sqrt{3} - 3\sqrt{6}}{10} B F(\alpha) G(\alpha).$$

In turn, the choice $A = 7$ and $B = 30$, Clausen's formula (10.19) (Proposition 10.4)

and

$$4t(1-t)\Big|_{t=(4\sqrt{2}-5\sqrt{3}+3)/(8\sqrt{2})} = -\frac{(\sqrt{3}-1)^6}{2^7}$$

imply

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} (7 + 30n) P_n\left(\frac{17}{12\sqrt{2}}\right) \left(\frac{-3}{4\sqrt{2}}\right)^n = \frac{\sqrt{6}(7\sqrt{3}-9)}{2} {}_3F_2\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \mid \frac{-(\sqrt{3}-1)^6}{2^7}\right)$$

$$+ \frac{9\sqrt{2}(101\sqrt{3}-175)}{128} {}_3F_2\left(\frac{3}{2}, \frac{3}{2}, \frac{3}{2} \mid \frac{-(\sqrt{3}-1)^6}{2^7}\right),$$

which is precisely $3/\sqrt{2}$ times the Ramanujan-type formula [30, eqn. (8.3)]

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^3}{n!^3} (7 - 3\sqrt{3} + 6(5 - \sqrt{3})n) \frac{(-1)^n(\sqrt{3} - 1)^{6n}}{2^{7n}} = \frac{4\sqrt{2}}{\pi}.$$

The derivation of (I4) is very similar, as the degree N is also 3 in this case (although we have to swap the rational p -parametric expressions of α and β). The choice of the parameter in the above rational parametrisation is $p = -(2 + \sqrt{3} + \sqrt{15})/4$, and the transformation (10.22) assumes the form

$$F\left(\frac{p(2+p)^3}{(1+2p)^3}\right) = -\frac{1+2p}{3} F\left(\frac{p^3(2+p)}{1+2p}\right) \quad \text{for } p \in (-\infty, -1).$$

This in fact follows from (10.22) by a change of variables then by applying to both sides a transformation of the complete elliptic integral K (as $K(t) = \pi F(t^2)/2$),

$$K(x) = \frac{1}{\sqrt{1-x^2}} K\left(\sqrt{\frac{x^2}{x^2-1}}\right), \tag{10.24}$$

itself a result of Euler’s hypergeometric transformation [25, §1.2, eqn. (2)].

Finally, (I4) reduces to Ramanujan’s identity [164, eqn. (30)]

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^3}{n!^3} (5\sqrt{5} - 1 + 6(7\sqrt{5} + 5)n) \frac{(\sqrt{5} - 1)^{8n}}{2^{14n}} = \frac{32}{\pi}.$$

For (I1) and (I3) we have to use the modular equations of degree 2 and 5, respectively [16, Chap. 19]; the corresponding “complex” Ramanujan-type series for $1/\pi$ required in the derivation of (I1) can be found in [108, Section 4].

Remark 10.3.1. When $s = 1/2$ we can take advantage of the functional equation

$$t\left(\tau + \frac{1}{2}\right) = \frac{t(\tau)}{t(\tau) - 1}, \tag{10.25}$$

which follows readily from Jacobi’s imaginary transformation [46] for K . Moreover,

$$F\left(\frac{t(\tau)}{t(\tau) - 1}\right) = F(t(\tau))\sqrt{1 - t(\tau)} \tag{10.26}$$

by Euler’s hypergeometric transformations. Therefore, aided by (10.25) and (10.26), we may carry out the same analysis as before for $\alpha = t(1/2 + \tau_0)$, $\beta = t(\tau_0/N)$, and a whole new range of identities follow.

For example, take $\tau_0 = \sqrt{-1/2}$ and $N = 1$ (a case not considered in Table 1), we have

$$\sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{4\sqrt{2} - 5}{7}\right) \left(\frac{5 - 3\sqrt{2}}{32}\right)^n (17 + 10(6 + \sqrt{2})n) = \frac{\sqrt{1282 + 922\sqrt{2}}}{\pi}, \tag{10.27}$$

while with $\tau_0 = i$ and $N = 2$, we produce the new rational series

$$\sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{2\sqrt{2}}{3}\right) \left(\frac{3\sqrt{2}}{128}\right)^n (6n+1) = \frac{2\sqrt{8+6\sqrt{2}}}{\pi}. \quad (10.28)$$

◇

10.4. Identities for $s = 1/3$

In this section we first prove (III1),

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} (2+15n) P_n\left(\frac{3\sqrt{3}}{5}\right) \left(\frac{5}{6\sqrt{3}}\right)^n = \frac{45\sqrt{3}}{4\pi},$$

which is representative of identities in the large group for $s = 1/3$ in Table 1. Here

$$\alpha = \frac{1 - \rho_0 - z_0}{2} = \frac{1}{4} \left(1 - \frac{1}{\sqrt{3}}\right)^3 \quad \text{and} \quad \beta = \frac{1 - \rho_0 + z_0}{2} = \frac{1}{2} \quad (10.29)$$

satisfy the modular equation of degree 2 in signature 3. Although a rational parametrisation similar to the one we exploited in Section 10.3 exists, we will compute the algebraic relations of Proposition 10.3 by using the modular equation itself

$$(\alpha\beta)^{1/3} + ((1-\alpha)(1-\beta))^{1/3} = 1, \quad (10.30)$$

as well as the equation for the corresponding multiplier [17, p. 120, Thm 7.1]

$$m = \frac{F(\beta)}{F(\alpha)} = \frac{(1-\alpha)^{2/3}}{(1-\beta)^{1/3}} - \frac{\alpha^{2/3}}{\beta^{1/3}}, \quad (10.31)$$

where $\alpha = \alpha(\tau) = t(\tau)$ has degree 2 over $\beta = \beta(\tau) = t(\tau/2)$.

On specialising (10.31) by taking $\tau = \tau_0$, we get

$$F\left(\frac{1}{2}\right) = \frac{2}{\sqrt{3}} F(\alpha)|_{\alpha=(1-1/\sqrt{3})^3/4}. \quad (10.32)$$

Computing the logarithmic t -derivative of (10.31) at $t = \alpha$, and using the notation of (10.5) result in

$$\begin{aligned} & \frac{G(\beta)}{\beta F(\beta)} \frac{d\beta}{d\alpha} - \frac{G(\alpha)}{\alpha F(\alpha)} = \frac{1}{m} \frac{d}{d\alpha} \left(\frac{(1-\alpha)^{2/3}}{(1-\beta)^{1/3}} - \frac{\alpha^{2/3}}{\beta^{1/3}} \right) \\ & = \frac{F(\alpha)}{F(\beta)} \frac{1}{3} \left(\frac{d\beta}{d\alpha} \left(\frac{(1-\alpha)^{2/3}}{(1-\beta)^{4/3}} + \frac{\alpha^{2/3}}{\beta^{4/3}} \right) - \frac{2}{(1-\alpha)^{1/3}(1-\beta)^{1/3}} - \frac{2}{\alpha^{1/3}\beta^{1/3}} \right). \end{aligned} \quad (10.33)$$

The derivative $d\beta/d\alpha$ can be obtained by differentiating (10.30),

$$\frac{d\beta}{d\alpha} \left(\frac{\alpha^{1/3}}{\beta^{2/3}} - \frac{(1-\alpha)^{1/3}}{(1-\beta)^{2/3}} \right) + \frac{\beta^{1/3}}{\alpha^{2/3}} - \frac{(1-\beta)^{1/3}}{(1-\alpha)^{2/3}} = 0,$$

so that

$$\left. \frac{d\beta}{d\alpha} \right|_{\tau=\tau_0} = 9.$$

Thus, with the choice $\tau = \tau_0$ in (10.33), we obtain

$$G\left(\frac{1}{2}\right) = \left(\frac{2}{9} F(\alpha) + \frac{3\sqrt{3} + 5}{3} G(\alpha) \right) \Big|_{\alpha=(1-1/\sqrt{3})^3/4}. \quad (10.34)$$

From now on we fix α and β as defined in (10.29). With the help of Proposition 10.2 and (10.32), (10.34) we find that

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} P_n(x_0) z_0^n &= F(\alpha) F(\beta) = \frac{2}{\sqrt{3}} F^2(\alpha), \\ \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} n P_n(x_0) z_0^n &= \frac{3\sqrt{3} + 5}{5} G(\alpha) F(\beta) + \frac{3\sqrt{3}}{5} F(\alpha) G(\beta) \\ &= \frac{2}{5\sqrt{3}} F^2(\alpha) + \frac{3\sqrt{3} + 5}{\sqrt{3}} F(\alpha) G(\alpha). \end{aligned}$$

Therefore,

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} (2 + 15n) P_n(x_0) z_0^n &= \frac{10}{\sqrt{3}} F^2(\alpha) + \frac{15(3\sqrt{3} + 5)}{\sqrt{3}} F(\alpha) G(\alpha) \\ &= \frac{5}{\sqrt{3}} \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{3})_n (\frac{2}{3})_n}{n!^3} (2 + 15n) (4\alpha(1 - \alpha))^n, \end{aligned}$$

while the latter is a multiple of Ramanujan's series [164, eqn. (31)]

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{3})_n (\frac{2}{3})_n}{n!^3} (2 + 15n) \left(\frac{2}{27}\right)^n = \frac{27}{4\pi},$$

and identity (III) follows.

Remark 10.4.1. In Section 10.8 we show that in the discussed example we have closed form evaluations of $F(1/2)$ and $G(1/2)$, hence of

$$F(\alpha) = \frac{\sqrt{3}}{2} F\left(\frac{1}{2}\right), \quad G(\alpha) = \frac{5\sqrt{3} - 9}{6} F\left(\frac{1}{2}\right) + \frac{9\sqrt{3} - 15}{2} G\left(\frac{1}{2}\right) \quad (10.35)$$

(the relations follow from (10.32) and (10.34)). In particular, this gives a different way of deducing (III), avoiding the use of a Ramanujan-type series. \diamond

We now turn our attention to (III1), shown below, for which $4|\alpha(1 - \alpha)| > 1$ and thus does not satisfy the conditions of Proposition 10.5. Our method employed is illustrative in dealing with more general situations when this occurs. It is also

worth noting that this approach bypasses the computational difficulties encountered with purely imaginary x_0 and z_0 (see Section 10.5), as is the case here.

We are required to prove

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} (2+9n) P_n \left(\frac{-7i\sqrt{5}}{22} \right) \left(\frac{-11i}{10\sqrt{5}} \right)^n = \frac{15\sqrt{3} + \sqrt{15}}{6\pi},$$

with $\alpha = (10\sqrt{5} - 27 + 11i)/(20\sqrt{5})$. We now take

$$p_0 = \frac{(1 + \sqrt{5})\sqrt{\sqrt{5} - 2} - \sqrt{22 - 10\sqrt{5}}}{4} - \frac{1}{2},$$

and apply the transformation [17, p. 112, Thm 5.6] or [46, Prop. 5.8]

$${}_2F_1 \left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| \frac{27p^2(1+p)^2}{4(1+p+p^2)^3} \right) = \frac{1+p+p^2}{\sqrt{1+2p}} {}_2F_1 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| \frac{p^3(2+p)}{1+2p} \right), \quad (10.36)$$

which is valid for real $p \in [0, 1)$. By analytic continuation, the transformation remains valid in a domain surrounding the origin in which the absolute values of the arguments of both hypergeometric functions are less than 1; in particular, this domain contains p_0 and its conjugate \bar{p}_0 .

In the notation

$$\tilde{F}(t) := {}_2F_1 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| t \right), \quad \tilde{G}(t) := t \frac{d}{dt} \tilde{F}(t),$$

the transformation (10.36) at $p = p_0$ gives

$$F(\alpha) = \frac{(2\sqrt{5} - 1 + (32 - 14\sqrt{5})i)^{1/4}}{\sqrt{2}} \tilde{F}(\alpha_0), \quad (10.37)$$

where $\alpha_0 = 1/2 - \sqrt{\sqrt{5} - 2}$ is real. Moreover, as β is the conjugate of α , it easily follows that at $p = \bar{p}_0$,

$$F(\beta) = \frac{(2\sqrt{5} - 1 - (32 - 14\sqrt{5})i)^{1/4}}{\sqrt{2}} \tilde{F}(\alpha_0). \quad (10.38)$$

Therefore, $F(\alpha)$ and $F(\beta)$ are both algebraic multiples of $\tilde{F}(\alpha_0)$, and we have transposed the problem to a simpler one in signature 2 with real argument. It remains to express $G(\alpha)$ and $G(\beta)$ in terms of $\tilde{F}(\alpha_0)$ and $\tilde{G}(\alpha_0)$.

To this end, we differentiate (10.36) with respect to p , and obtain

$$\begin{aligned} & \frac{(1-p)(2+p)(1+2p)^{5/2}}{(1+p)(1+p+p^2)} G \left(\frac{27p^2(1+p)^2}{4(1+p+p^2)^3} \right) \\ &= 3p^2(1+p) \tilde{F} \left(\frac{p^3(2+p)}{1+2p} \right) + \frac{6(1+p)^2(1+p+p^2)}{2+p} \tilde{G} \left(\frac{p^3(2+p)}{1+2p} \right). \end{aligned} \quad (10.39)$$

Substituting p_0 and its complex conjugate \bar{p}_0 , respectively, into (10.39) simplifies both $G(\alpha)$ and $G(\beta)$ in terms of the desired functions. Armed with this knowledge as well as with (10.37) and (10.38), we can use Proposition 10.2 to obtain

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} (2 + 9n) P_n \left(\frac{-7i\sqrt{5}}{22} \right) \left(\frac{-11i}{10\sqrt{5}} \right)^n \\ &= \frac{\sqrt{5} \sqrt{41\sqrt{5} - 89}}{\sqrt{6}} \tilde{F}^2(\alpha_0) + \left(\frac{5(\sqrt{3} + 3\sqrt{5})}{6} + \frac{10\sqrt{17\sqrt{5} - 31}}{\sqrt{6}} \right) \tilde{F}(\alpha_0) \tilde{G}(\alpha_0). \end{aligned}$$

This now satisfies the conditions of Proposition 10.4 with $s = 1/2$, and the truth of (III1) is reduced to that of a classical Ramanujan series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^3}{n!^3} (5 - \sqrt{5} + 20n) \left(\frac{\sqrt{5} - 1}{2} \right)^{6n} = \frac{2\sqrt{5}}{\pi} \sqrt{2 + \sqrt{5}}, \tag{10.40}$$

as $4\alpha_0(1 - \alpha_0) = ((\sqrt{5} - 1)/2)^6$ – we comment on this numerical coincidence in Section 10.8.

Remark 10.4.2. We note that six of the identities in group II in Table 1, as well as (A1) and (A2), satisfy $\tau_0 = \sqrt{-2p/3}$, where $\mathbb{Q}(\sqrt{-2p/3})$ has class number 4; therefore $p \in \{5, 7, 13, 17\}$. That these series are rational could be attributed to this observation. \diamond

10.5. Identities for $s = 1/4$

Although in this section we focus on the proof of identity (III5),

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n (\frac{3}{4})_n}{n!^2} (13 + 80n) P_n \left(-\frac{7i}{33\sqrt{15}} \right) \left(-\frac{11i\sqrt{15}}{147} \right)^n = \frac{7\sqrt{42}(3 + 2\sqrt{5})}{8\pi},$$

and on our new “rational” identity (10.50), it is worth commenting on the proof of (III3) first, which is very similar to the one of (II1) presented in Section 10.4.

Example 10.5.1. For (III3) we get

$$\alpha = \frac{(\sqrt{6} - 2)^4}{2^3 \cdot 7^2}, \quad \beta = \frac{1}{2},$$

the degree 3 modular equation reads

$$(\alpha\beta)^{1/2} + ((1 - \alpha)(1 - \beta))^{1/2} + 4(\alpha\beta(1 - \alpha)(1 - \beta))^{1/4} = 1, \tag{10.41}$$

while the underlying series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{4})_n (\frac{3}{4})_n}{n!^3} \frac{3 + 40n}{7^{4n}} = \frac{1}{3\pi\sqrt{3}}$$

is due to Ramanujan [164, eqn. (42)]. A more elementary derivation of (III1), which we discuss in Section 10.8, is also available for (III3). \diamond

In the case of (III5), we have $\tau_0 = (1 + i\sqrt{15})/4$, $N = 2$,

$$\alpha = t(\tau_0) = \frac{1}{2} - \frac{32\sqrt{5}}{3 \cdot 7^2} + \frac{11i\sqrt{15}}{6 \cdot 7^2}, \quad \beta = \frac{1}{2} - \frac{32\sqrt{5}}{3 \cdot 7^2} - \frac{11i\sqrt{15}}{6 \cdot 7^2},$$

and $\beta' = 1 - \beta = t(\tau_0/2)$. Note that for subsequent calculations,

$$\beta^{1/2} = \frac{4\sqrt{5} - 5}{14} - i \frac{\sqrt{15} + 4\sqrt{3}}{42}.$$

The degree 2 modular equation for $s = 1/4$ is [69, eqn. (4.6)]

$$\alpha^{1/2}(1 + 3(1 - \beta')^{1/2}) = 1 - (1 - \beta')^{1/2}, \quad (10.42)$$

and the multiplier is given by [69, eqn. (4.5)]

$$m = \frac{F(\beta')}{F(\alpha)} = 2(1 + 3(1 - \beta')^{1/2})^{-1/2}. \quad (10.43)$$

Using (10.16) and (10.42), we can find the ratio between $F(\beta')$ and $F(\beta)$, as well as between $F(\beta')$ and $F(\alpha)$:

$$F(\beta) = \frac{3 + 2\sqrt{5} - (\sqrt{5} - 2)\sqrt{3}i}{2\sqrt{14}} F(\alpha), \quad (10.44)$$

$$F(\beta') = \frac{2\sqrt{3} + \sqrt{15} + (2\sqrt{5} - 3)i}{2\sqrt{7}} F(\alpha). \quad (10.45)$$

Relation (10.18) of Proposition 10.3 assumes the form

$$G(\beta) = \frac{(7 - 3\sqrt{5})(5\sqrt{15} + 61i)}{128\sqrt{2}} G(\beta') + \frac{3(69 + 7\sqrt{5}) + 33i\sqrt{3}(15 - 7\sqrt{5})}{256\sqrt{2}\pi} F(\beta'). \quad (10.46)$$

It remains to express $G(\beta')$ as a linear combination of $G(\alpha)$ and $F(\alpha)$. Proceeding in a similar fashion as Section 10.4 (for (II1)), we differentiate both sides of (10.42) with respect to t at α , and obtain

$$(1 + 3\beta^{1/2})^2 \beta^{1/2} = (1 - \beta^{1/2} + 3\alpha(1 + 3\beta^{1/2})) \frac{d\beta'}{d\alpha},$$

from which we easily solve for $d\beta'/d\alpha$; this we substitute into the next equation, obtained by differentiating both sides of (10.43):

$$G(\beta') = \frac{\beta' G(\alpha) F(\beta')}{\alpha F(\alpha)} \left(\frac{d\beta'}{d\alpha} \right)^{-1} + \frac{3\beta' F(\alpha)}{2\beta^{1/2}(1 + 3\beta^{1/2})^{3/2}}. \quad (10.47)$$

Now (10.47), when tidied up via (10.45), expresses $G(\beta')$ in terms of $G(\alpha)$ and $F(\alpha)$ as promised. Substituting the result into (10.46) and using (10.45) again,

after much computational work we arrive at an expression of $G(\beta)$ in terms of $G(\alpha)$ and $F(\alpha)$:

$$G(\beta) = \frac{3\sqrt{7}(23\sqrt{15} - 39\sqrt{3} - (3\sqrt{5} + 1)i)}{256\sqrt{2}\pi F(\alpha)} - \frac{15 + 18\sqrt{5} + (38\sqrt{3} - 23\sqrt{15})i}{112\sqrt{14}} F(\alpha) - \frac{513 + 323\sqrt{5} + (153\sqrt{3} - 361\sqrt{15})i}{448\sqrt{14}} G(\alpha). \quad (10.48)$$

Combining (10.44) and (10.48) with Proposition 10.2 allows us to invoke Proposition 10.4 to arrive at a series equivalent to (III5); the corresponding Ramanujan-type series and its conjugate are given by

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{4})_n (\frac{3}{4})_n}{n!^3} ((52 \mp 12i\sqrt{3}) + (320 \mp 55i\sqrt{3})n) \left(\frac{2(5 \pm i\sqrt{3})}{7\sqrt{3}} \right)^{4n} = \frac{98\sqrt{3}}{\pi}, \quad (10.49)$$

as we have

$$4\alpha(1 - \alpha) = \left(\frac{2(5 + i\sqrt{3})}{7\sqrt{3}} \right)^4$$

in this case.

Remark 10.5.1. We remark that the Ramanujan-type series (10.49) are *rational* over the ring $\mathbb{Z}[e^{2\pi i/3}]$. A possible way to establish them rests upon application of degree 2 modular equations (10.42), (10.43) with the different choice

$$\alpha = t \left(\frac{i\sqrt{15} \pm 1}{2} \right) = - \left(\frac{16 - 7\sqrt{5}}{11\sqrt{3}} \right)^2, \quad \beta' = t \left(\frac{i\sqrt{15} \pm 1}{4} \right),$$

so that α is *real*, and on using the *real* Ramanujan-type series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{4})_n (\frac{3}{4})_n}{n!^3} (1500 - 604\sqrt{5} + (6825 - 2240\sqrt{5})n) \times (-1)^n \left(\frac{2(13 - 5\sqrt{5})}{11\sqrt{3}} \right)^{4n} = \frac{121\sqrt{15}}{\pi}$$

for the argument $4\alpha(1 - \alpha)$; this is very similar to what was done for (III1) in Section 10.4. A different approach is to apply the general construction in Section 10.10. \diamond

We now present some new *rational* series that are analogous to (III2). Our first series for $s = 1/4$ corresponds to the choice

$$x_0 = \frac{199}{60\sqrt{11}}, \quad z_0 = \frac{-5\sqrt{11}}{96}, \quad \rho_0 = \frac{65}{32\sqrt{3}}, \quad \tau_0 = \frac{i\sqrt{33} + 3}{2}, \quad \text{and} \quad N = 3,$$

in the notation of Table 1. Then we have

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n (\frac{3}{4})_n}{n!^2} (33 + 260n) P_n(x_0) z_0^n = \frac{32\sqrt{6}}{\pi},$$

or alternatively in the form involving T_n (as in (10.1)),

$$\sum_{n=0}^{\infty} \frac{33 + 260n}{(-384^2)^n} \binom{4n}{2n} \binom{2n}{n} T_n(398, 1) = \frac{32\sqrt{6}}{\pi}. \quad (10.50)$$

The proof proceeds in the fashion of (III1) via the degree 3 modular equation and the multiplier in signature 4 (see [17, pp. 153–154]), and the Ramanujan-type series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n (\frac{3}{4})_n (\frac{1}{2})_n}{n!^3} (33\sqrt{33} - 119 + (260\sqrt{33} - 220)n) \left(\frac{325\sqrt{33} - 1867}{4608} \right)^n = \frac{128\sqrt{3}}{\pi}.$$

The three other new series are obtained by choosing

$$\tau_0 \in \left\{ \frac{i\sqrt{57} + 3}{2}, \frac{i\sqrt{93} + 3}{2}, \frac{i\sqrt{177} + 3}{2} \right\}$$

and, again, $N = 3$. They are:

$$\sum_{n=0}^{\infty} \frac{7\,331 + 83\,980n}{(-2\,688^2)^n} \binom{4n}{2n} \binom{2n}{n} T_n(2\,702, 1) = \frac{80\sqrt{42^3}}{\pi}, \quad (10.51)$$

$$\sum_{n=0}^{\infty} \frac{71\,161 + 1\,071\,980n}{(-24\,288^2)^n} \binom{4n}{2n} \binom{2n}{n} T_n(24\,302, 1) = \frac{135\sqrt{253^3}}{\pi\sqrt{6}}, \quad (10.52)$$

$$\sum_{n=0}^{\infty} \frac{30\,282\,753 + 632\,736\,260n}{(-1\,123\,584^2)^n} \binom{4n}{2n} \binom{2n}{n} T_n(1\,123\,598, 1) = \frac{2944\sqrt{1463^3}}{\pi\sqrt{3}}. \quad (10.53)$$

The partial sum of (10.53) adds about four digits of accuracy per term.

In order to find these new series similar to (III2), we search for imaginary quadratic fields $\mathbb{Q}(\sqrt{-3\ell})$ with class number 4, where prime $\ell \equiv 3 \pmod{4}$. It turns out that this is satisfied when $\ell = 7, 11, 19, 31$ and 59 (this list seems exhaustive). The four new series correspond to the latter four discriminants, respectively.

Another curious observation is that, in the notation of

$$\sum_{n=0}^{\infty} \frac{A + Bn}{\Lambda^n} \binom{4n}{2n} \binom{2n}{n} T_n(b, 1) = \frac{C}{\pi},$$

when $N = 3$ we have $|b - |\Lambda|^{1/2}| = 14$. This is observed in (III1)–(III3), as well as in (10.50)–(10.53), and in fact follows from the modular equation (10.41).

Remark 10.5.2. In a more recent version of his preprint [183], Sun gives eight new series for group III. Not surprisingly, these too are subsumed under our theory. Indeed, for all of them, $\tau_0 = \sqrt{-pq/2}$ and the underlying quadratic field again has

class number 4 (so $p = 5, 7, 13$ or 17 , and all of Sun's cases have $q = 3$). Using other values of q , we may produce many more rational series. As just one example, with $\tau_0 = \sqrt{-35/2}$ and $N = 5$, we have

$$\sum_{n=1}^{\infty} \frac{(\frac{1}{4})_n (\frac{3}{4})_n}{n!^2} (17 + 230n) P_n \left(\frac{19601}{13860\sqrt{2}} \right) \left(\frac{110\sqrt{2}}{567} \right)^n = \frac{135\sqrt{21}}{4\sqrt{2}\pi}. \quad (10.54)$$

Our next example, not found by Sun, is the following, which has $\tau = \sqrt{-7}$ and $N = 2$:

$$\sum_{n=1}^{\infty} \frac{(\frac{1}{4})_n (\frac{3}{4})_n}{n!^2} (841 + 9520n) P_n \left(\frac{4097}{4095} \right) \left(\frac{455}{29241} \right)^n = \frac{513\sqrt{114}}{2\pi}. \quad (10.55)$$

◇

10.6. New identities for $s = 1/6$

In this section, we illustrate two series corresponding to $s = 1/6$, a case not considered in [183].

Our first example follows by taking $\tau_0 = i\sqrt{6}$ and $N = 2$. Then

$$\frac{1728}{j(\tau_0)} = \frac{1399 - 988\sqrt{2}}{4913} \quad \text{and} \quad \frac{1728}{j(\tau_0/2)} = \frac{1399 + 988\sqrt{2}}{4913},$$

and we have two Ramanujan-type series of Proposition 10.5,

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{6})_n (\frac{5}{6})_n}{n!^3} (5 + 12(5 \mp \sqrt{2})n) \left(\frac{1399 \pm 988\sqrt{2}}{4913} \right)^n = \frac{3 \pm 1}{2\pi} \sqrt{213 \mp 24\sqrt{2}}.$$

Note that adding these two series gives a rational left-hand side. By using either of the two series, and with

$$x_0 = \frac{17\sqrt{17} - 46}{2\sqrt{1757 - 391\sqrt{17}}}, \quad z_0 = \frac{\sqrt{1757 - 391\sqrt{17}}}{17\sqrt{17}},$$

we obtain

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{6})_n (\frac{5}{6})_n}{n!^2} (5(31 + 17\sqrt{17}) + 5928n) P_n(x_0) z_0^n = \frac{17\sqrt{6}}{\pi} \sqrt{1069\sqrt{17} - 1683}. \quad (10.56)$$

In the second example we choose $\tau_0 = i\sqrt{7} + 1$ and $N = 2$, so that

$$\frac{1728}{j(\tau_0)} = \left(\frac{4}{85} \right)^3 \quad \text{and} \quad \frac{1728}{j(\tau_0/2)} = -\left(\frac{4}{5} \right)^3,$$

and the related Ramanujan-type series is

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (\frac{1}{6})_n (\frac{5}{6})_n}{n!^3} (8 + 133n) \left(\frac{4}{85} \right)^{3n} = \frac{\sqrt{85^3}}{18\pi\sqrt{3}},$$

due to Ramanujan himself [164, eqn. (34)]. The series and the corresponding choice

$$x_0 = \frac{323\sqrt{1785}}{13650} - \frac{\sqrt{105}}{40950}, \quad z_0 = \frac{171\sqrt{1785}}{14450} - \frac{3\sqrt{105}}{50}$$

generate the formula

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{6}\right)_n \left(\frac{5}{6}\right)_n}{n!^2} (1687 - 15\sqrt{17^3} + 6552n) P_n(x_0) z_0^n = \frac{85\sqrt{30}}{32\pi} \sqrt{19809\sqrt{17} - 68425}.$$

In notation of (10.1), the identity can be stated in the form

$$\begin{aligned} \sum_{n=0}^{\infty} \binom{6n}{3n} \binom{3n}{n} (1687 - 15\sqrt{17^3} + 6552n) T_n\left(\frac{10773 - 125\sqrt{17^3}}{32}, -1\right) \frac{1}{(-15\sqrt{17})^{3n}} \\ = \frac{85\sqrt{30}}{32\pi} \sqrt{19809\sqrt{17} - 68425}. \end{aligned} \quad (10.57)$$

The appearance of a negative c in (10.1) is not found on the list from [183].

Remark 10.6.1. Note that given τ_0 and N , formulas such as (10.56) can be experimentally discovered using PSLQ, working in the Gaussian integers if one needs to. More specifically, if one suspects the existence of a series of the type

$$(a + b\sqrt{k})F^2(t_0) + (c + d\sqrt{k})F(t_0)G(t_0) = \frac{\sqrt{e + f\sqrt{k}}}{\pi},$$

where $a, b, c, d, e, f \in \mathbb{Q}$ and k is often a factor of an integer appearing in the surd of τ_0 , then one could evaluate $F(t_0)$, $G(t_0)$ to very high precision, and run PSLQ on the square of the series. That is, with $F_1 = F^2(t_0)$ and $F_2 = F(t_0)G(t_0)$, one would run PSLQ on the vector

$$\left\{ F_1^2, \sqrt{k}F_1^2, F_2^2, \sqrt{k}F_2^2, F_1F_2, \sqrt{k}F_1F_2, \frac{1}{\pi^2}, \frac{\sqrt{k}}{\pi^2} \right\}.$$

Some of the identities in this chapter were first found this way; generalisations and improvements of this method are also possible. \diamond

10.7. Companion series

If we differentiate (10.4) with respect to x instead of z , a series involving the derivatives of Legendre polynomials is obtained:

Proposition 10.6. *In the notation of (10.5),*

$$\sum_{n=0}^{\infty} \frac{(s)_n (1-s)_n}{n!^2} P'_n(x) z^n = z \left(\frac{G(t_-)F(t_+)}{1-\rho-z} + \frac{F(t_-)G(t_+)}{1-\rho+z} \right), \quad (10.58)$$

where $t_{\pm} = t_{\pm}(x, z) := (1 - \rho \pm z)/2$.

We may then take a linear combination of the series (10.6) and (10.58), and apply Proposition 10.4 to match a series for $1/\pi$ (of the type in Proposition 10.5), thus obtaining what we call a “companion series”.

For instance, in the case of (III), the resulting companion series is

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{3}\right)_n \left(\frac{2}{3}\right)_n}{n!^2} \left[P'_n \left(\frac{3\sqrt{3}}{5} \right) + \sqrt{3} P_n \left(\frac{3\sqrt{3}}{5} \right) \right] \left(\frac{5}{6\sqrt{3}} \right)^n = \frac{15}{2\pi}.$$

If we combine (III), its companion, and the formula [196, Ch. 15]

$$P'_n(x) = \frac{n}{x^2 - 1} (xP_n(x) - P_{n-1}(x)), \quad (10.59)$$

we produce the new identity

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{3}\right)_n \left(\frac{2}{3}\right)_n}{n!^2} n P_{n-1} \left(\frac{3\sqrt{3}}{5} \right) \left(\frac{5}{6\sqrt{3}} \right)^n = \frac{3}{4\pi}.$$

Note that the second order recursion satisfied by P_n (14.25) allows us to derive many identities of this kind.

As another example of a companion series, (I4) produces

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{n!^2} \left[\frac{7}{26\sqrt{5}} P'_n \left(\frac{31}{8\sqrt{15}} \right) + \frac{214}{13\sqrt{3}} P_n \left(\frac{31}{8\sqrt{15}} \right) \right] \left(\frac{\sqrt{15}}{16} \right)^n = \frac{32}{\pi}.$$

10.8. Closed forms

Here we give our elementary proof of (III) as promised in Remark 10.4.1. Using the same notation as Section 10.4, applying Proposition 10.2 and relation (10.35), we obtain

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{3}\right)_n \left(\frac{2}{3}\right)_n}{n!^2} (2 + 15n) P_n \left(\frac{3\sqrt{3}}{5} \right) \left(\frac{5}{6\sqrt{3}} \right)^n = \frac{45}{2} F \left(\frac{1}{2} \right) G \left(\frac{1}{2} \right).$$

Note that both the hypergeometric series on the right-hand side can be summed by Gauss’ second summation theorem [25, §2.4, eqn. (2)]:

$$F \left(\frac{1}{2} \right) = {}_2F_1 \left(\frac{1}{3}, \frac{2}{3} \mid \frac{1}{2} \right) = \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{2}{3})\Gamma(\frac{5}{6})}, \quad G \left(\frac{1}{2} \right) = \frac{1}{9} {}_2F_1 \left(\frac{4}{3}, \frac{5}{3} \mid \frac{1}{2} \right) = \frac{2\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{3})\Gamma(\frac{1}{6})}.$$

Therefore,

$$F \left(\frac{1}{2} \right) G \left(\frac{1}{2} \right) = \frac{\sqrt{3}}{2\pi},$$

and identity (III) follows. As mentioned, a similar derivation is valid for (III3).

When $s = 1/2$, we can alternatively use the complete elliptic integrals K and K' to represent proofs of the identities in group I. This sometimes leads to closed form evaluations of the involved $F(\alpha)$ and $F(\beta)$, hence also of $G(\alpha)$ and $G(\beta)$ through the corresponding series for $1/\pi$ or by taking derivatives. Our evaluations depend on the N th singular value of K , that is, a modulus k_N such that $\frac{K'(k_N)}{K(k_N)} = \sqrt{N}$. For a positive integer N , k_N is algebraic and can be effectively computed [164], and the values of K and its derivative at k_N (hence $F(k_N^2)$ and $G(k_N^2)$) are expressible in terms of gamma functions (see [46, Ch. 5], which also lists k_N for small N).

Consider, for example, the product $F(\alpha)F(\beta)$ for (I2); with the help of (10.22) we see that it is

$$\frac{2\sqrt{6}(\sqrt{3}+1)}{3\pi^2} K^2\left(\sqrt{\frac{4\sqrt{2}-5\sqrt{3}-3}{8\sqrt{2}}}\right).$$

We now apply the transformation (10.24) followed by the quadratic transform (6.5), and observe that the argument of the elliptic integral is transformed to k'_3 , where $k_3 = \sin(\pi/12)$ is the third singular value. As $K'(k_3)$ has a closed form, we obtain

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} P_n\left(\frac{17}{12\sqrt{2}}\right) \left(-\frac{3}{4\sqrt{2}}\right)^n = \frac{3\Gamma(\frac{1}{3})^6}{2^{11/3}\pi^4}.$$

Curiously enough, the quantity on the right-hand side is exactly the value of $W_3(-1)$ in Chapter 1.

In (I3) and (I4), $\alpha = 16 - 7\sqrt{3} - \sqrt{15}$ is the square of the 15th singular value of K . In the proof of (III1), α_0 is the square of the fifth singular value. In all these cases, F and G all have computable closed forms at α and α_0 ; we can therefore complete their proofs without resorting to Propositions 10.4 and 10.5. In the case of (III1) we can use this fact to establish the series (10.40).

10.9. Summary

We have discussed the proofs of several Ramanujan-type series for $1/\pi$ that are associated with the Legendre polynomials. Our analysis in Sections 10.5 and 10.6 shows that the list in [183] does not exhaust all, even rational, examples of such series, and that the latter problem is related to investigation of imaginary quadratic fields with prescribed class groups. In particular, our work effectively gives a recipe to generate more series of the type by picking suitable τ in imaginary quadratic fields.

The techniques of the present chapter also allow us to prove other identities in [183] of the forms

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} (A + Bn) P_{2n}(x_0) z_0^n = \frac{C}{\pi} \quad \text{and} \quad \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} (A + Bn) P_{3n}(x_0) z_0^n = \frac{C}{\pi}, \quad (10.60)$$

although computation becomes more involved. Brafman's generating function (10.4) in these cases is replaced by new generating functions in [193] (Chapter 11). In the next section, we return to an encountered complex series for $1/\pi$ and give explicit details for its construction.

10.10. Complex Series for $1/\pi$

Almost all currently known series for $1/\pi$ share one common property that the coefficients are all real. In [108], J. Guillera and W. Zudilin discovered the first series for $1/\pi$ with complex coefficients, namely,

$$\sum_{k=0}^{\infty} \frac{(\frac{1}{2})_k^3}{k!^3} \left(\frac{49 - 13\sqrt{-7}}{64} + \frac{105 - 21\sqrt{-7}}{32} k \right) \left(\frac{47 + 45\sqrt{-7}}{128} \right)^k = \frac{\sqrt{7}}{\pi}. \quad (10.61)$$

This series was shown to be equivalent to another series involving only real numbers, and the proof of the latter follows from the Wilf-Zeilberger method.

In Section 10.5, we encountered two series analogous to (10.61), namely,

$$\sum_{k=0}^{\infty} \frac{(\frac{1}{2})_k (\frac{1}{4})_k (\frac{3}{4})_k}{k!^3} (52 \pm 12\sqrt{-3} + (320 \mp 55\sqrt{-3})k) \left(\frac{2(5 \pm \sqrt{-3})}{7\sqrt{3}} \right)^{4k} = \frac{98\sqrt{3}}{\pi}. \quad (10.62)$$

It suffices to prove any one of the above series since one is the conjugate of the other. Here, we will discuss a general method to establish identities such as (10.62).

10.10.1. Functions associated with $\Gamma_0(2)$. Series such as (10.62) arise from Ramanujan's quartic theory of elliptic functions [36]. We recall some of the facts from [36]. For $|q| < 1$, define

$$f(-q) = \prod_{j=1}^{\infty} (1 - q^j).$$

When $q = e^{2\pi i\tau}$ with $\text{Im } \tau > 0$, we find that

$$q^{1/24} f(-q) = \eta(\tau),$$

where $\eta(\tau)$ is the Dedekind η -function already encountered in Chapters 3 and 7. It is well known [12, Theorem 3.1] that $\eta(\tau)$ satisfies the transformation

$$\eta\left(-\frac{1}{\tau}\right) = \sqrt{-i\tau} \eta(\tau). \quad (10.63)$$

Let

$$Z(q) = \frac{f^8(-q) + 32qf^8(-q^4)}{f^4(-q^2)} \quad \text{and} \quad X(q) = 4x(q)(1 - x(q)), \quad (10.64)$$

where

$$\frac{1}{x(q)} = 1 + \frac{f^{24}(-q)}{64qf^{24}(-q^2)}. \quad (10.65)$$

In [36], we know that

$$Z(q) = {}_3F_2\left(\begin{matrix} \frac{1}{4}, \frac{3}{4}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| X(q)\right).$$

To extract π from these functions, we need the transformation formula which follows from (10.63). More precisely, we have

$$Z\left(e^{2\pi i\left(\frac{-1}{\sqrt{2}\tau}\right)}\right) = -\tau^2 Z\left(e^{2\pi i\tau/\sqrt{2}}\right).$$

Differentiating the above with respect to τ , we deduce that

$$\frac{1}{\tau} \cdot \frac{q}{Z} \frac{dZ}{dq} \Big|_{q=e^{-2\pi i/(\sqrt{2}\tau)}} = \frac{\sqrt{2}}{\pi i} + \tau \cdot \frac{q}{Z} \frac{dZ}{dq} \Big|_{q=e^{2\pi i\tau/\sqrt{2}}}.$$

To simplify notations, let

$$G(\tau) = \frac{q}{Z} \frac{dZ}{dq} \Big|_{q=e^{2\pi i\tau/\sqrt{2}}}.$$

Then the transformation can be rewritten as

$$\frac{1}{\tau} G\left(-\frac{1}{\tau}\right) = \frac{\sqrt{2}}{\pi i} + \tau G(\tau). \quad (10.66)$$

Note the appearance of π . In the next subsection, we will express $G(\tau)$ and $G(-1/\tau)$ in terms of a hypergeometric function and its derivative.

In the case of series for $1/\pi$ with real coefficients, we would only need one modular equation. To prove (10.62), we will see that *two* modular equations are needed.

10.10.2. Some intermediate identities. Set

$$\tau_1 = \frac{\sqrt{-15} - 1}{2\sqrt{2}}, \quad \tau_2 = \frac{\sqrt{-5/3} - 1}{2\sqrt{2}}, \quad \text{and} \quad \tau_3 = \frac{\sqrt{-15} + 1}{2\sqrt{2}}. \quad (10.67)$$

From (10.66), we deduce that

$$G\left(-\frac{1}{\tau_1}\right) = \tau_1 \frac{\sqrt{2}}{\pi i} - \left(\frac{7}{4} + \frac{\sqrt{-15}}{4}\right) G(\tau_1)$$

and

$$G(\tau_2) = \left(\frac{1}{\tau_2}\right)^2 G(\tau_1) + \frac{1}{\tau_2} \frac{\sqrt{2}}{\pi i},$$

where we have used $-1/\tau_2 = \tau_1 + \sqrt{2}$, which implies that

$$G\left(-\frac{1}{\tau_2}\right) = G(\tau_1).$$

Hence, we find that

$$G\left(-\frac{1}{\tau_1}\right) = \frac{\sqrt{-15} - 1}{2\pi i} - \left(\frac{7}{4} + \frac{\sqrt{-15}}{4}\right) G(\tau_1), \quad (10.68)$$

$$G(\tau_2) = \left(-\frac{3}{4} + \frac{3}{4}\sqrt{-15}\right) G(\tau_1) + \left(-\frac{3}{2} - \frac{1}{2}\sqrt{-15}\right) \frac{1}{\pi i}. \quad (10.69)$$

Now, let

$$M_N(q) = \frac{Z(q)}{Z(q^N)}, \quad (10.70)$$

Then we find that

$$\frac{q}{M_N(q)} \frac{dM_N(q)}{dq} = \tilde{Z}(q) - N\tilde{Z}(q^N), \quad \text{where} \quad \tilde{Z}(q) = \frac{q}{Z(q)} \frac{dZ(q)}{dq}.$$

Letting $q = e^{2\pi i\tau/\sqrt{2}}$, this implies

$$G(\tau) - NG(N\tau) = \tilde{M}_N(\tau), \quad \text{where} \quad \tilde{M}_N(\tau) = \frac{q}{M_N(q)} \frac{dM_N(q)}{dq}. \quad (10.71)$$

When $N = 2$, we have

$$G\left(-\frac{1}{\tau_1}\right) - 2G(\tau_3) = \tilde{M}_2\left(-\frac{1}{\tau_1}\right) \quad (10.72)$$

and when $N = 3$,

$$G(\tau_2) - 3G(\tau_3) = \tilde{M}_3(\tau_2). \quad (10.73)$$

Note how the judicious choices of τ_1 , τ_2 and τ_3 allow us to derive these identities relating G at τ_i . Using (10.68), (10.69), (10.72) and (10.73), we could eliminate $G(-\frac{1}{\tau_1})$ and $G(\tau_2)$ to obtain two equations relating $G(\tau_1)$ and $G(\tau_3)$. Using these two equations to eliminate $G(\tau_1)$ or $G(\tau_3)$, we would arrive at the two complex

series for $1/\pi$. It remains to compute the right hand side of (10.72) and (10.73) explicitly, which is achieved in (10.78) and (10.79) below.

10.10.3. Modular equations of degree 2 and 3. A modular equation of degree N is a relation between $x(q)$ and $x(q^N)$, where $x(q)$ is given by (10.65). We will need the following modular equations in signature 4:

Proposition 10.7. *Let $\alpha = x(q)$ and $\gamma = x(q^2)$. Then*

$$64\gamma - 80\gamma\alpha + 18\gamma\alpha^2 - 81\gamma^2\alpha^2 + 144\gamma^2\alpha - 64\gamma^2 - \alpha^2 = 0. \quad (10.74)$$

Proposition 10.8. *Let $\alpha = x(q)$ and $\beta = x(q^3)$. Then*

$$\begin{aligned} &\alpha^4 + \beta^4 + 141056\beta^3\alpha^3 + 19206\beta^2\alpha^2 - 4096\alpha\beta + 36864\beta^4\alpha^4 \\ &- 3972(\beta^3\alpha + \alpha^3\beta) + 36480(\alpha^4\beta^2 + \beta^4\alpha^2) - 73728(\beta^4\alpha^3 + \alpha^4\beta^3) \\ &+ 384(\alpha^4\beta + \beta^4\alpha) + 7680(\alpha^2\beta + \beta^2\alpha) - 63360(\alpha^3\beta^2 + \beta^3\alpha^2) = 0. \end{aligned} \quad (10.75)$$

Let $F(\tau) = x(q)$, with $q = e^{2\pi i\tau/\sqrt{2}}$. We first find $F(\tau_i)$. Since

$$3\tau_2 = \tau_3 - \sqrt{2},$$

we find that $F(\tau_2)$ and $F(\tau_3)$ satisfy (10.75). In a similar way, we conclude that $F(-1/\tau_1)$ and $F(\tau_3)$ satisfies (10.74). Now, using (10.63), we find that

$$F\left(-\frac{1}{\tau_1}\right) = 1 - F(\tau_1).$$

We also deduce that

$$F(\tau_2) = 1 - F\left(-\frac{1}{\tau_2}\right) = 1 - F(\tau_1), \quad (10.76)$$

where we have used $-\frac{1}{\tau_2} = \tau_1 + \sqrt{2}$. We have obtained enough equations to solve for $F(\tau_i)$. Solving them, we conclude that

$$F(\tau_1) = \frac{1}{2} - \frac{32}{147}\sqrt{5} - \frac{11}{294}\sqrt{-15}.$$

By taking the conjugate, we find that

$$F(\tau_3) = \frac{1}{2} - \frac{32}{147}\sqrt{5} + \frac{11}{294}\sqrt{-15}.$$

By (10.76), we deduce that

$$F(\tau_2) = \frac{1}{2} + \frac{32}{147}\sqrt{5} + \frac{11}{294}\sqrt{-15}.$$

We next obtain an expression for M_N defined by (10.70). It is known [36] that for a positive integer N ,

$$q^N \frac{dx(q^N)}{d(q^N)} = \frac{Z(q^N)}{4} X(q^N),$$

where X is defined by (10.64). This yields

$$M_N = \frac{1}{N} \frac{dx(q)}{dx(q^N)} \frac{X(q^N)}{X(q)}. \quad (10.77)$$

But if we are given a modular equation of degree N , then the right hand side of (10.77) can be expressed in terms of $X(q)$ and $X(q^N)$. We can then derive an explicit expression of $dM_N/dX(q)$ in terms of $X(q)$ and $X(q^N)$, and this in turn yields the expression for \widetilde{M}_N defined by (10.71). We carry out these computations and determine the right hand side of (10.72). Differentiating (10.74) with respect to α , we conclude that

$$\frac{d\gamma}{d\alpha} = \frac{80\gamma - 36\gamma\alpha + 162\gamma^2\alpha - 144\gamma^2 + 2\alpha}{64 - 80\alpha + 18\alpha^2 - 162\gamma\alpha^2 + 288\gamma\alpha - 128\gamma}.$$

Hence,

$$M_2 = \frac{1}{2} \frac{64 - 80\alpha + 18\alpha^2 - 162\gamma\alpha^2 + 288\gamma\alpha - 128\gamma}{80\gamma - 36\gamma\alpha + 162\gamma^2\alpha - 144\gamma^2 + 2\alpha} \frac{\gamma(1-\gamma)}{\alpha(1-\alpha)}.$$

Differentiating M_2 with respect to α , and letting $\alpha = F(-1/\tau_1)$ and $\gamma = F(\tau_3)$, we conclude that

$$G\left(-\frac{1}{\tau_1}\right) - 2G(\tau_3) = \left(\frac{11}{49} + \frac{\sqrt{5}}{7} + \frac{\sqrt{-15}}{21} - \frac{\sqrt{-3}}{147}\right) Z(\tau_1). \quad (10.78)$$

In a similar way, we use (10.75) and the relation between $Z(\tau_1) = Z(-1/\tau_2)$ and $Z(\tau_2)$ to deduce from (10.73) that

$$G(\tau_2) - 3G(\tau_3) = \left(\frac{4}{49}\sqrt{5} - \frac{20}{49}\sqrt{-3} + \frac{2}{49}\sqrt{-15} + \frac{30}{49}\right) Z(\tau_1). \quad (10.79)$$

Next, using (10.68) and (10.69) in (10.78) and (10.79), we find that

$$\left(\frac{15}{4} + \frac{9}{4}\sqrt{-15}\right) G(\tau_1) + \left(\frac{27}{49} - \frac{13}{49}\sqrt{5} - \frac{3}{49}\sqrt{-15} - \frac{39}{49}\sqrt{-3}\right) Z(\tau_1) = \frac{9i + \sqrt{15}}{2\pi}.$$

Finally, observing that

$$Z(\tau_1) = \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}\right)_k \left(\frac{1}{4}\right)_k \left(\frac{3}{4}\right)_k}{k!^3} (4F(\tau_1)(1-F(\tau_1)))^k,$$

$$G(\tau_1) = (1-2F(\tau_1)) \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}\right)_k \left(\frac{1}{4}\right)_k \left(\frac{3}{4}\right)_k}{k!^3} k (4F(\tau_1)(1-F(\tau_1)))^k,$$

we obtain the desired series for $1/\pi$.

Remark 10.10.1. The degrees of modular equations to be used to prove complex series for $1/\pi$ are not as obvious as in the real series. In the real series for $1/\pi$, if $\tau = \sqrt{-pq/2}$ where p and q are primes, then it is clear that we need modular equations of degree p and q . In the complex case, we observe that the squares of the *norms* of

$$\frac{1}{\sqrt{2}} \frac{\tau_3}{(-1/\tau_1)} \quad \text{and} \quad \frac{1}{\sqrt{2}} \frac{\tau_3}{\tau_2}$$

are 2 and 3, respectively. These norms determine the degrees of modular equations we used. The method presented here can also be applied to complex series for $1/\pi$ in other alternative bases. \diamond

Remark 10.10.2. A different approach to derive complex series for $1/\pi$ is based on transformations of hypergeometric series; the required details of the method can be found in [75]. For instance, again starting from (10.40), using the transformation (10.36) and the generating function

$$\sum_{k=0}^{\infty} \delta_k u^k = \frac{1}{1-4u} {}_3F_2 \left(\begin{matrix} \frac{1}{3}, \frac{1}{2}, \frac{2}{3} \\ 1, 1 \end{matrix} \middle| \frac{108u^2}{(1-4u)^3} \right)$$

of the *Domb numbers* [75] (which also appear as $W_4(2k)$ in Chapter 3) at $u = (3 - 2i - \sqrt{5 - 10i})/32$, we obtain the following two *complex* series:

$$\begin{aligned} & \sum_{k=0}^{\infty} \frac{(\frac{1}{3})_k (\frac{1}{2})_k (\frac{2}{3})_k}{k!^3} (3(401 - i - (109 - 69i)\sqrt{1+2i}) + 5830k) \\ & \times \left(\frac{27(2530 + 1451i - 65(30 - i)\sqrt{1+2i})}{495 - 4888i} \right)^k = \frac{3321 - 381i + 81(33 - 17i)\sqrt{1+2i}}{4\pi}, \\ & \sum_{k=0}^{\infty} (69 + 13i - (23 - 7i)\sqrt{1+2i} + 170k) \delta_k \left(\frac{3 - 2i - (1 - 2i)\sqrt{1+2i}}{32} \right)^k \\ & = \frac{66 + 42i + 12(1 - 4i)\sqrt{1+2i}}{\pi}. \end{aligned}$$

Similarly, a complex series may also be obtained for the Apéry numbers, used in the irrationality proof of $\zeta(3)$ [187]. These arithmetically significant sequences are the higher order analogs of the Apéry-like sequences used in Chapter 11. Another complex series can be seen in (12.35). \diamond

# in [183]	s	x_0	z_0	ρ_0	A	B	C	τ_0	N
(I1)*	1/2	$\frac{-i}{3\sqrt{7}}$	$\frac{-3i\sqrt{7}}{16}$	$\frac{15}{16}$	7	30	24	$\frac{i\sqrt{7}+1}{4}$	2
(I2)	1/2	$\frac{17}{12\sqrt{2}}$	$\frac{-3}{4\sqrt{2}}$	$\frac{5\sqrt{3}}{4\sqrt{2}}$	7	30	12	$\frac{2i\sqrt{3}-3}{2}$	3
(I3)	1/2	$\frac{97}{56\sqrt{3}}$	$\frac{7\sqrt{3}}{16}$	$\frac{\sqrt{15}}{16}$	-1	30	80	$\frac{i\sqrt{15}}{2}$	5
(I4)	1/2	$\frac{31}{8\sqrt{15}}$	$\frac{\sqrt{15}}{16}$	$\frac{7\sqrt{3}}{16}$	5	42	$16\sqrt{3}$	$\frac{i\sqrt{15}}{2}$	3
(II1)	1/3	$\frac{3\sqrt{3}}{5}$	$\frac{5}{6\sqrt{3}}$	$\frac{5}{6\sqrt{3}}$	2	15	$\frac{45\sqrt{3}}{4}$	$\frac{2i}{\sqrt{3}}$	2
(II2)	1/3	$\frac{5}{2\sqrt{6}}$	$\frac{27\sqrt{3}}{125\sqrt{2}}$	$\frac{91}{125}$	12	91	$\frac{75\sqrt{3}}{2}$	$i\sqrt{2}$	2
(II3)	1/3	$\frac{99}{70\sqrt{2}}$	$\frac{35}{27\sqrt{2}}$	$\frac{\sqrt{5}}{27}$	-4	15	$\frac{135\sqrt{3}}{2}$	$\frac{i\sqrt{10}}{\sqrt{3}}$	5
(II4)	1/3	$\frac{485}{198\sqrt{6}}$	$\frac{99\sqrt{3}}{125\sqrt{2}}$	$\frac{\sqrt{14}}{125}$	-41	42	$525\sqrt{3}$	$\frac{i\sqrt{14}}{\sqrt{3}}$	7
(II5)	1/3	$\frac{365}{364}$	$\frac{91}{125}$	$\frac{27\sqrt{3}}{125\sqrt{2}}$	1	18	$25\sqrt{3}$	$i\sqrt{2}$	3
(II6)	1/3	$\frac{51}{10\sqrt{26}}$	$\frac{5\sqrt{13}}{4913\sqrt{2}}$	$\frac{3465\sqrt{2}}{4913}$	559	6930	$\frac{1445\sqrt{6}}{2}$	$\frac{i\sqrt{26}}{\sqrt{3}}$	2
(II7)	1/3	$\frac{99}{70\sqrt{2}}$	$\frac{35}{35937\sqrt{2}}$	$\frac{8710\sqrt{17}}{35937}$	15724	222105	$\frac{114345\sqrt{3}}{4}$	$\frac{i\sqrt{34}}{\sqrt{3}}$	2
(II8)	1/3	$\frac{19601}{13860\sqrt{2}}$	$\frac{3465\sqrt{2}}{4913}$	$\frac{5\sqrt{13}}{4913\sqrt{2}}$	-3967	390	$56355\sqrt{3}$	$\frac{i\sqrt{26}}{\sqrt{3}}$	13
(II9)	1/3	$\frac{143649}{34840\sqrt{17}}$	$\frac{8710\sqrt{17}}{35937}$	$\frac{35}{35937\sqrt{2}}$	-7157	210	$114345\sqrt{3}$	$\frac{i\sqrt{34}}{\sqrt{3}}$	17
(II10)*	1/3	$\frac{-13i}{4\sqrt{35}}$	$\frac{i\sqrt{35}}{64}$	$\frac{27\sqrt{5}}{64}$	7	45	$\frac{8(3+\sqrt{5})}{\sqrt{3}}$	$\frac{i\sqrt{35}-1}{6}$	3
(II11)*	1/3	$\frac{-7i\sqrt{5}}{22}$	$\frac{-11i}{10\sqrt{5}}$	$\frac{27}{10\sqrt{5}}$	2	9	$\frac{15+\sqrt{5}}{2\sqrt{3}}$	$\frac{i\sqrt{5}+1}{3}$	2
(II12)*	1/3	$\frac{-10i\sqrt{2}}{23}$	$\frac{-23i}{125\sqrt{2}}$	$\frac{189}{125\sqrt{2}}$	11	63	$\frac{25(3+4\sqrt{2})}{4\sqrt{3}}$	$\frac{i\sqrt{8}+1}{3}$	3
(A1)	1/3	$\frac{9}{4\sqrt{5}}$	$\frac{\sqrt{5}}{27}$	$\frac{35}{27\sqrt{2}}$	5	42	$\frac{54\sqrt{3}}{5}$	$\frac{i\sqrt{10}}{\sqrt{3}}$	2
(A2)	1/3	$\frac{15}{4\sqrt{14}}$	$\frac{\sqrt{14}}{125}$	$\frac{99\sqrt{3}}{125\sqrt{2}}$	7	66	$\frac{50\sqrt{2}}{3}$	$\frac{i\sqrt{14}}{\sqrt{3}}$	2
(III1)	1/4	$\frac{52}{30\sqrt{3}}$	$\frac{160}{121\sqrt{3}}$	$\frac{85}{363}$	2	85	$33\sqrt{33}$	$i\sqrt{3}$	3
(III2)	1/4	$\frac{55}{12\sqrt{21}}$	$\frac{-\sqrt{21}}{6}$	$\frac{2\sqrt{7}}{3}$	5	28	$3\sqrt{6}$	$\frac{i\sqrt{21}+3}{2}$	3
(III3)	1/4	$\frac{49}{20\sqrt{6}}$	$\frac{10\sqrt{6}}{49}$	$\frac{10\sqrt{6}}{49}$	3	40	$\frac{70\sqrt{21}}{9}$	$\frac{3i}{\sqrt{2}}$	3
(III4)	1/4	$\frac{257}{255}$	$\frac{85}{363}$	$\frac{160}{121\sqrt{3}}$	9	80	$\frac{11\sqrt{66}}{2}$	$i\sqrt{3}$	2
(III5)*	1/4	$\frac{-7i}{33\sqrt{15}}$	$\frac{-11i\sqrt{15}}{147}$	$\frac{64\sqrt{5}}{147}$	13	80	$\frac{7\sqrt{42}(3+2\sqrt{5})}{8}$	$\frac{i\sqrt{15}+1}{4}$	2

TABLE 1. Identities (10.3), and the corresponding choice of τ_0 and N such that $(1 - \rho_0 - z_0)/2 = t(\tau_0)$ and $(1 - \rho_0 + z_0)/2 = t(\tau_0/N)$ or $1 - t(\tau_0/N)$ (the latter is for entries marked by an asterisk).

Generating Functions of Legendre Polynomials

ABSTRACT. In 1951, F. Brafman derived several “unusual” generating functions of orthogonal polynomials, in particular, of the Legendre polynomials $P_n(x)$. His result was a consequence of Bailey’s identity for a special case of Appell’s hypergeometric function. In this chapter, we present a generalisation of Bailey’s identity and its implication to generating functions of the form $\sum_{n=0}^{\infty} u_n P_n(x) z^n$, where u_n is an Apéry-like sequence, that is, a sequence satisfying $(n+1)^2 u_{n+1} = (an^2 + an + b)u_n - cn^2 u_{n-1}$ where $u_{-1} = 0$, $u_0 = 1$. Using our results, we also give generating functions for rarefied Legendre polynomials and construct a new family of identities for $1/\pi$.

11.1. Introduction

The Legendre polynomials,

$$\begin{aligned} P_n(x) &= {}_2F_1\left(\begin{matrix} -n, n+1 \\ 1 \end{matrix} \middle| \frac{1-x}{2}\right) = \left(\frac{x+1}{2}\right)^n {}_2F_1\left(\begin{matrix} -n, -n \\ 1 \end{matrix} \middle| \frac{x-1}{x+1}\right) \\ &= \sum_{m=0}^n \binom{n}{m}^2 \left(\frac{x-1}{2}\right)^m \left(\frac{x+1}{2}\right)^{n-m}, \end{aligned} \tag{11.1}$$

admit many generating functions. One particular family shown below is due to Fred Brafman in 1951, which, as shown in our previous work [74] (Chapter 10), finds some nice applications in number theory, namely, in constructing new Ramanujan-type formulas for $1/\pi$.

Theorem A (Brafman [63]). *The following generating function is valid:*

$$\sum_{n=0}^{\infty} \frac{(s)_n (1-s)_n}{n!^2} P_n(x) z^n = {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| \frac{1-\rho-z}{2}\right) \cdot {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| \frac{1-\rho+z}{2}\right), \tag{11.2}$$

where $\rho = (1 - 2xz + z^2)^{1/2}$.

Theorem A in the form

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} P_n\left(\frac{X+Y-2XY}{Y-X}\right) (Y-X)^n \\ &= {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| X\right) \cdot {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| Y\right) \end{aligned} \quad (11.3)$$

is derived in [63] as a consequence of Bailey's identity for a special case of Appell's hypergeometric function of the fourth type [25, Section 9.6],

$$\begin{aligned} & \sum_{m,k=0}^{\infty} \frac{(s)_{m+k}(1-s)_{m+k}}{m!^2 k!^2} (X(1-Y))^m (Y(1-X))^k \\ &= {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| X\right) \cdot {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| Y\right). \end{aligned} \quad (11.4)$$

We note that by specialising $Y = X$, one recovers a particular case of Clausen's formula:

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, s, 1-s \\ 1, 1 \end{matrix} \middle| 4X(1-X)\right) = {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| X\right)^2.$$

Remark 11.1.1. The region where (11.3) holds is somewhat subtle for real X and Y : it is the open region bounded by $X + Y = 1$, $Y = X + 1$, $Y = X - 1$, and the lower branch of the hyperbola $X^2 - 6XY + Y^2 + 2X + 2Y + 1 = 0$. When $X = Y$, the left-hand side of (11.3) is understood as the limit as $X \rightarrow Y$. \diamond

In 1959 Brafman addressed a different type of generating function; the results wherein were later generalised by H. M. Srivastava in [182, eqn. (37)].

Theorem B (Brafman [64], Srivastava [182]). *For a positive integer N , a (generic) sequence $\lambda_0, \lambda_1, \dots$ and a complex number w ,*

$$\frac{1}{\rho} \sum_{k=0}^{\infty} \lambda_k P_{Nk} \left(\frac{x-z}{\rho} \right) \left(w \frac{z^N}{\rho^N} \right)^k = \sum_{n=0}^{\infty} A_n P_n(x) z^n,$$

where $\rho = (1 - 2xz + z^2)^{1/2}$ and

$$A_n = A_n(w) = \sum_{k=0}^{\lfloor n/N \rfloor} \binom{n}{Nk} \lambda_k w^k.$$

Brafman's original results in [64] concern the cases $N = 1, 2$ and a sequence λ_n given as a quotient of Pochhammer symbols (λ_n is called a *hypergeometric term*).

In this chapter we extend Bailey's identity (11.4) to more general Apéry-like sequences u_0, u_1, u_2, \dots which satisfy the second order recurrence relation

$$(n+1)^2 u_{n+1} = (an^2 + an + b)u_n - cn^2 u_{n-1} \quad \text{for } n = 0, 1, 2, \dots, \quad u_{-1} = 0, u_0 = 1, \quad (11.5)$$

for given a, b and c .

Our first result concerns the generating function of u_n . It is the main theorem of this chapter, and captures a wide range of series for $1/\pi$; an attempt to illustrate its relationships with other theorems is found in Figure 1.

Theorem 11.1. *For the solution u_n of the recurrence equation (11.5), define*

$$g(X, Y) = \frac{X(1 - aY + cY^2)}{(1 - cXY)^2}. \quad (11.6)$$

Then in a neighbourhood of $X = Y = 0$,

$$\left\{ \sum_{n=0}^{\infty} u_n X^n \right\} \left\{ \sum_{n=0}^{\infty} u_n Y^n \right\} = \frac{1}{1 - cXY} \sum_{n=0}^{\infty} u_n \sum_{m=0}^n \binom{n}{m}^2 g(X, Y)^m g(Y, X)^{n-m}. \quad (11.7)$$

We remark that the generating function $F(X) = \sum_{n=0}^{\infty} u_n X^n$ for a sequence satisfying (11.5) is a unique, analytic-at-the-origin solution of the differential equation

$$(\theta^2 - X(a\theta^2 + a\theta + b) + cX^2(\theta + 1)^2)F(X) = 0, \quad \text{where } \theta = \theta_X := X \frac{\partial}{\partial X}. \quad (11.8)$$

The hypergeometric term $u_n = (s)_n(1-s)_n/n!^2$ corresponds to a special degenerate case $c = 0$ and $a = 1, b = s(1-s)$ in (11.5). Therefore, Bailey's identity (11.4) corresponds to the particular choice $c = 0$ in Theorem 11.1.

Theorem 11.1 also generalises Clausen-type formulas given in [72] which arise as specialisation $Y = X$; see Section 11.2 for details.

Following Brafman's derivation of Theorem A in [63] we deduce the following generalised generating function of Legendre polynomials.

Theorem 11.2. For the solution u_n of the recurrence equation (11.5), the following identity is valid in a neighbourhood of $X = Y = 0$:

$$\begin{aligned} & \sum_{n=0}^{\infty} u_n P_n \left(\frac{(X+Y)(1+cXY) - 2aXY}{(Y-X)(1-cXY)} \right) \left(\frac{Y-X}{1-cXY} \right)^n \\ &= (1-cXY) \left\{ \sum_{n=0}^{\infty} u_n X^n \right\} \left\{ \sum_{n=0}^{\infty} u_n Y^n \right\}. \end{aligned} \quad (11.9)$$

Finally, combining the results of Theorem B and Theorem 11.2 we construct two new generating functions of rarefied Legendre polynomials.

Theorem 11.3. The following identities are valid in a neighbourhood of $X = Y = 1$:

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} P_{2n} \left(\frac{(X+Y)(1-XY)}{(X-Y)(1+XY)} \right) \left(\frac{X-Y}{1+XY} \right)^{2n} \\ &= \frac{1+XY}{2} {}_2F_1 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| 1-X^2 \right) {}_2F_1 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| 1-Y^2 \right), \end{aligned} \quad (11.10)$$

and

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} P_{3n} \left(\frac{X+Y-2X^2Y^2}{(X-Y)\sqrt{1+4XY(X+Y)}} \right) \left(\frac{X-Y}{\sqrt{1+4XY(X+Y)}} \right)^{3n} \\ &= \frac{\sqrt{1+4XY(X+Y)}}{3} {}_2F_1 \left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| 1-X^3 \right) {}_2F_1 \left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| 1-Y^3 \right). \end{aligned} \quad (11.11)$$

As an application of Theorems 11.2 and 11.3, we outline proofs of Ramanujan type series for $1/\pi$ experimentally observed by Z.-W. Sun in [183], as well as of several new ones; this is addressed in Section 11.5. In Section 11.2 we discuss arithmetic sequences that solve the recursion (11.5). Our proofs of Theorems 11.1–11.3 are given in Sections 11.3 and 11.4.

11.2. Apéry-like sequences

Although our Theorems 11.1 and 11.2 are true for generic (a, b, c) in (11.5), there are fourteen (up to normalisation) non-degenerate examples when the sequence u_n satisfies (11.5) and takes *integral* values. These were first listed by D. Zagier in [200] (see also [8]), and the generating functions of all these sequences are known to have a *modular* parametrisation. Table 1 indicates the related data for the sequences; the first four examples are hypergeometric ($c = 0$), the next four are known as

# in [8]	# in [200]	(a, b, c)	u_n
(A)	#11	$(16, 4, 0)$	$\binom{2n}{n}^2$
(B)	#14	$(27, 6, 0)$	$\binom{2n}{n} \binom{3n}{n}$
(C)	#20	$(64, 12, 0)$	$\binom{2n}{n} \binom{4n}{2n}$
(D)		$(432, 60, 0)$	$\binom{3n}{n} \binom{6n}{3n}$
(e)	#19	$(32, 12, 16^2)$	$16^n \sum_{k=0}^n (-1)^k \binom{-\frac{1}{2}}{k} \binom{-\frac{1}{2}}{n-k}^2$
(h)	#25	$(54, 21, 27^2)$	$27^n \sum_{k=0}^n (-1)^k \binom{-\frac{2}{3}}{k} \binom{-\frac{1}{3}}{n-k}^2$
(i)	#26	$(128, 52, 64^2)$	$64^n \sum_{k=0}^n (-1)^k \binom{-\frac{3}{4}}{k} \binom{-\frac{1}{4}}{n-k}^2$
(j)		$(864, 372, 432^2)$	$432^n \sum_{k=0}^n (-1)^k \binom{-\frac{5}{6}}{k} \binom{-\frac{1}{6}}{n-k}^2$
(a)	#5, A	$(7, 2, -8)$	$\sum_{k=0}^n \binom{n}{k}^3$
(b)	#9, D	$(11, 3, -1)$	$\sum_{k=0}^n \binom{n}{k}^2 \binom{n+k}{n}$
(c)	#8, C	$(10, 3, 9)$	$\sum_{k=0}^n \binom{n}{k}^2 \binom{2k}{k}$
(d)	#10, E	$(12, 4, 32)$	$\sum_{k=0}^n \binom{n}{k} \binom{2k}{k} \binom{2(n-k)}{n-k}$
(f)	#7, B	$(9, 3, 27)$	$\sum_{k=0}^{\lfloor n/3 \rfloor} (-1)^k 3^{n-3k} \binom{n}{3k} \frac{(3k)!}{(k!)^3}$
(g)	#13, F	$(17, 6, 72)$	$\sum_{k=0}^n \binom{n}{k} (-1)^k 8^{n-k} \sum_{j=0}^k \binom{k}{j}^3$

TABLE 1. Arithmetic solutions of (11.5).

Legendrian examples ($a^2 - 4c = 0$), while the remaining six cases are so-called ‘sporadic’ examples in the terminology of [200]. Note that for the hypergeometric examples, Theorem 11.2 reduces precisely to special cases of Theorem A investigated in Chapter 10.

We remark that our Theorem 11.2 for the Legendrian cases (entries (e), (h), (i), and (j) in Table 1) follows from Theorem A applied to hypergeometric instances (A)–(D) and Theorem B with choice $N = 1$; this is because the Legendrian and

hypergeometric cases are related by a *binomial transform*. Moreover, entries (a) and (c) as well as (a) and (g) are also related by similar transforms and so are connected by Theorem B; for example, the first pair is related by the identity

$$\sum_{k=0}^n \binom{n}{k} \sum_{j=0}^k \binom{k}{j}^3 = \sum_{k=0}^n \binom{n}{k}^2 \binom{2k}{k}.$$

Note however that Theorem 11.2 is stronger, since it works for any sequence satisfying the recursion (11.5).

We also recall that if $f(x)$, $g(x)$ are the generating functions of two sequences related by a binomial transform, then

$$g(x) = \frac{1}{1-x} f\left(\frac{x}{x-1}\right), \quad (11.12)$$

which we implicitly use in Section 11.5.

Remark 11.2.1. The sequence (e) is very interesting as it has many equivalent expressions as ${}_3F_2$'s, such as

$$u_n^{(e)} = 16^n {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, -n \\ 1, 1 \end{matrix} \middle| 1\right).$$

Perhaps because of this, Brafman was able to anticipate our Theorem 11.2 for (e). In [64], he gave

$$\sum_{n=0}^{\infty} P_n(x) u_n^{(e)} \left(\frac{z}{16}\right)^n = \frac{1}{\rho} {}_2F_1\left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| \frac{\rho-1+z}{2\rho}\right) {}_2F_1\left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| \frac{\rho-1-z}{2\rho}\right).$$

◇

The following general Clausen-type formula was shown in [72].

Proposition 11.1. For the solution u_n of the recurrence equation (11.5),

$$\left\{ \sum_{n=0}^{\infty} u_n X^n \right\}^2 = \frac{1}{1-cX^2} \sum_{n=0}^{\infty} u_n \binom{2n}{n} \left(\frac{X(1-aX+cX^2)}{(1-cX^2)^2} \right)^n. \quad (11.13)$$

Because $g(X, X) = X(1-aX+cX^2)/(1-cX^2)^2$ for the function $g(X, Y)$ defined in (11.6) and

$$\sum_{k=0}^n \binom{n}{k}^2 = \binom{2n}{n},$$

identity (11.13) follows from taking $Y = X$ in Theorem 11.1. However, Proposition 11.1 is the result which suggested to us the form of Theorem 11.1.

Discussions of why the six sporadic examples are arithmetically important, as well as details of modular parametrisations of the corresponding generating functions $\sum_{n=0}^{\infty} u_n X^n$ can be found in [8], [71], [72], and [200]. Our new series for $1/\pi$ in Section 11.5 are consequences of the above knowledge and our Theorem 11.2.

11.3. Generalised Bailey's identity

We begin by proving our main theorem, which generalises Bailey's identity.

PROOF OF THEOREM 11.1. First, define the two-variable generating function

$$H(x, y) := \sum_{n=0}^{\infty} u_n \sum_{m=0}^n \binom{n}{m}^2 x^m y^{n-m} \tag{11.14}$$

and the linear differential operator

$$\begin{aligned} \Delta_{x,y} := & (c(x^2 + 6xy + y^2) - a(x + y) + 1) \left(x \frac{\partial^2}{\partial x^2} + y \frac{\partial^2}{\partial y^2} \right) \\ & + 4xy(2c(x + y) - a) \frac{\partial^2}{\partial x \partial y} + (c(5x^2 + 14xy + y^2) - a(3x + y) + 1) \frac{\partial}{\partial x} \\ & + (c(x^2 + 14xy + 5y^2) - a(x + 3y) + 1) \frac{\partial}{\partial y} + 2(c(x + y) - b). \end{aligned} \tag{11.15}$$

Applying the operator (11.15) to (11.14) and rearranging the summation over monomials, we find that (after a lot of elementary algebra)

$$\Delta_{x,y} H = 2 \sum_n ((n + 1)^2 u_{n+1} - (an^2 + an + b)u_n + cn^2 u_{n-1}) \sum_m \binom{n}{m}^2 x^m y^{n-m} = 0 \tag{11.16}$$

because of the recurrence equation (11.5).

Secondly, the one-variable differential operator

$$\begin{aligned} D_X := & X(1 - aX + cX^2) \frac{\partial^2}{\partial X^2} + (1 - 2aX + 3cX^2) \frac{\partial}{\partial X} + (cX - b) \\ = & X^{-1}(\theta_X^2 - X(a\theta_X^2 + a\theta_X + b) + cX^2(\theta_X + 1)^2) \end{aligned}$$

annihilates the series $F(X) := \sum_{n=0}^{\infty} u_n X^n$ by (11.8), therefore

$$(D_X + D_Y)(F(X)F(Y)) = 0. \tag{11.17}$$

On the other hand, we find after some work that

$$\begin{aligned} & (1 - cXY)(D_X + D_Y) \left(\frac{1}{1 - cXY} H(g(X, Y), g(Y, X)) \right) \\ & = (\Delta_{x,y} H(x, y)) \Big|_{x=g(X,Y), y=g(Y,X)}, \end{aligned}$$

and the latter vanishes by (11.16). Comparing this result with (11.17) we conclude that both $F(X)F(Y)$ and $H(g(X, Y), g(Y, X))/(1 - cXY)$ satisfy the same second order linear partial differential equation $(D_X + D_Y)G(X, Y) = 0$. By straightforward verification, these two (analytic at the origin) solutions agree as functions of X when $Y = 0$; we claim that they in fact coincide, and Theorem 11.1 follows.

To verify the claim, consider the function

$$G(X, Y) := F(X)F(Y) - \frac{H(g(X, Y), g(Y, X))}{1 - cXY},$$

which is analytic at the origin, is annihilated by $D_X + D_Y$, and satisfies $G(X, 0) = 0$. The latter condition implies that in the power series

$$G(X, Y) = \sum_{m,k} v_{m,k} X^m Y^k = \sum_{m,k=0}^{\infty} v_{m,k} X^m Y^k$$

we have $v_{m,0} = 0$ for all m . Applying $D_X + D_Y$ to the series, we obtain

$$\begin{aligned} \sum_{m,k} ((m+1)^2 v_{m+1,k} - (am^2 + am + b)v_{m,k} + cm^2 v_{m-1,k} \\ + (k+1)^2 v_{m,k+1} - (ak^2 + ak + b)v_{m,k} + ck^2 v_{m,k-1}) X^m Y^k = 0. \end{aligned} \quad (11.18)$$

Now, assuming that $v_{m,k} = 0$ for all m and all $k \leq k'$ and substituting $k = k'$ into (11.18), we readily see that $v_{m,k'+1} = 0$ for all m . It thus follows by induction on k that $v_{m,k} = 0$ for all m and k , that is, G is identically zero. \square

Remark 11.3.1. We did *not* find the operator $\Delta_{x,y}$ in (11.15) from D_X or D_Y using a change of variables, since for generic a and c , X and Y are very complicated functions of x and y . Instead, we used repeated experiments on particular values of a and c , and managed to *guess* the coefficients in $\Delta_{x,y}$ one at a time.

We are glad to learn that the proof of Theorem 11.1 has been subsequently fully computerised (A. Bostan, P. Lairez and B. Salvy, private communication via W. Zudilin, June 2012). \diamond

11.4. Generating functions of Legendre polynomials

Theorem 11.1 paves way for an easy proof of our next result.

PROOF OF THEOREM 11.2. The application of (11.7) follows the lines of deducing Brafman’s formula (11.2) from Bailey’s reduction formula (11.4): using representation (11.1) for Legendre polynomials, write

$$\sum_{n=0}^{\infty} u_n P_n(x) z^n = \sum_{n=0}^{\infty} u_n \sum_{m=0}^n \binom{n}{m}^2 \left(\frac{z(x-1)}{2}\right)^m \left(\frac{z(x+1)}{2}\right)^{n-m}$$

and choose X and Y in (11.7) to satisfy

$$\begin{aligned} \frac{z(x-1)}{2} &= g(X, Y) = \frac{X(1-aY+cY^2)}{(1-cXY)^2}, \\ \frac{z(x+1)}{2} &= g(Y, X) = \frac{Y(1-aX+cX^2)}{(1-cXY)^2}. \end{aligned} \tag{11.19}$$

One easily solves (11.19) with respect to x and z :

$$x = \frac{(X+Y)(1+cXY) - 2aXY}{(Y-X)(1-cXY)}, \quad z = \frac{Y-X}{1-cXY},$$

and identity (11.9) follows. □

By taking $N = 2$, $\lambda_k = (\frac{1}{2})_k^2/k!^2$, and $w = 1$ in Theorem B, we obtain

Proposition 11.2.

$$\frac{1}{\rho} \sum_{k=0}^{\infty} \frac{(\frac{1}{2})_k^2}{k!^2} P_{2k} \left(\frac{x-z}{\rho}\right) \left(\frac{z}{\rho}\right)^{2k} = \sum_{n=0}^{\infty} v_n P_n(x) \left(\frac{z}{4}\right)^n, \tag{11.20}$$

where

$$v_n = 4^n \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{2k} \frac{(\frac{1}{2})_k^2}{k!^2} = \sum_{k=0}^n \binom{n}{k} \binom{2k}{k} \binom{2(n-k)}{n-k}.$$

A different choice of $N = 3$, $\lambda_k = (\frac{1}{3})_k (\frac{2}{3})_k / k!^2$, and $w = -1$ in Theorem B results in

Proposition 11.3.

$$\frac{1}{\rho} \sum_{k=0}^{\infty} \frac{(\frac{1}{3})_k (\frac{2}{3})_k}{k!^2} P_{3k} \left(\frac{x-z}{\rho}\right) \left(-\frac{z}{\rho}\right)^{3k} = \sum_{n=0}^{\infty} w_n P_n(x) \left(\frac{z}{3}\right)^n, \tag{11.21}$$

where

$$w_n = \sum_{k=0}^{\lfloor n/3 \rfloor} (-1)^k 3^{n-3k} \binom{n}{3k} \frac{(3k)!}{(k!)^3}.$$

We are now in a position to prove Theorem 11.3.

PROOF OF THEOREM 11.3. Write identity (11.20) in the form

$$\sum_{n=0}^{\infty} v_n P_n(x) z^n = \frac{1}{\rho_2} \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}\right)_k^2}{k!^2} P_{2k} \left(\frac{x-4z}{\rho_2} \right) \left(\frac{4z}{\rho_2} \right)^{2k}, \quad (11.22)$$

where $\rho_2 = \rho_2(x, z) := (1 - 8xz + 16z^2)^{1/2}$, and apply Theorem 11.2 to the left-hand side of (11.22) and the sequence $v_n = u_n^{(d)}$ (entry (d) in Table 1) to get

$$\left\{ \sum_{n=0}^{\infty} v_n X^n \right\} \left\{ \sum_{n=0}^{\infty} v_n Y^n \right\} = \sum_{k=0}^{\infty} \binom{2k}{k}^2 P_{2k} \left(\frac{(1-4X-4Y)(X+Y-8XY)}{(Y-X)(1-4X-4Y+32XY)} \right) \times \frac{(X-Y)^{2k}}{(1-4X-4Y+32XY)^{2k+1}}. \quad (11.23)$$

To each of the factors on the left-hand side we can further apply

$$\sum_{n=0}^{\infty} v_n X^n = {}_2F_1 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| 16X(1-4X) \right)$$

to reduce (11.23) to a hypergeometric form. Finally, making the change of variables $X \mapsto (1-X)/8$, $Y \mapsto (1-Y)/8$ we arrive at (11.10).

For the second identity in Theorem 11.3, write (11.21) as

$$\sum_{n=0}^{\infty} w_n P_n(x) z^n = \frac{1}{\rho_3} \sum_{k=0}^{\infty} \frac{\left(\frac{1}{3}\right)_k \left(\frac{2}{3}\right)_k}{k!^2} P_{3k} \left(\frac{x-3z}{\rho_3} \right) \left(-\frac{3z}{\rho_3} \right)^{3k}, \quad (11.24)$$

where $\rho_3 = \rho_3(x, z) := (1 - 6xz + 9z^2)^{1/2}$. Then apply Theorem 11.2 to the left-hand side of (11.24) and the sequence $w_n = u_n^{(f)}$, use

$$\sum_{n=0}^{\infty} w_n X^n = \frac{1}{1-9X} {}_2F_1 \left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| -\frac{27X(1-9X+27X^2)}{(1-9X)^3} \right),$$

and make the change of variables $X \mapsto (X-1)/(9X)$, $Y \mapsto (Y-1)/(9Y)$ in the resulting identity. (The generating function above is easily checkable using the differential equation (11.8).) This gives us (11.11). \square

11.5. Formulas for $1/\pi$

We briefly recall our general strategy in Chapter 10 for proving identities for $1/\pi$. Suppose that we have a functional identity of the form

$$\sum_{n=0}^{\infty} u_n P_{\ell n}(x) z^n = \gamma F(\alpha) F(\beta), \quad (11.25)$$

where $\ell \in \{1, 2, 3\}$, and α , β and γ are algebraic functions of x and z (Theorems A, 11.2 and 11.3 are sources of such identities). Computing the z -derivative of both sides of (11.25) results in

$$\sum_{n=0}^{\infty} u_n n P_{\ell n}(x) z^n = \gamma_0 F(\alpha) F(\beta) + \gamma_1 F(\alpha) G(\beta) + \gamma_2 G(\alpha) F(\beta), \quad (11.26)$$

where γ_0 , γ_1 and γ_2 are algebraic functions of x and z . We take algebraic $x = x_0$ and $z = z_0$ in (11.25) and (11.26) such that the corresponding quantities $\alpha = \alpha(x_0, z_0)$ and $\beta = \beta(x_0, z_0)$ are values of a modular function $t(\tau)$ at quadratic irrationalities: $\alpha = t(\tau_0)$, and $\beta = t(\tau_0/N)$ or $1 - t(\tau_0/N)$ for an integer N . Using the modular equation of degree N , we can always express $F(\beta)$ and $G(\beta)$ by means of $F(\alpha)$ and $G(\alpha)$ only:

$$F(\beta) = \mu_0 F(\alpha) \quad \text{and} \quad G(\beta) = \lambda_0 F(\alpha) + \lambda_1 G(\alpha) + \frac{\lambda_2}{\pi F(\alpha)}, \quad (11.27)$$

where μ_0 , λ_0 , λ_1 , and λ_2 are algebraic ($\lambda_2 = 0$ when $\beta = t(\tau_0/N)$). Substituting relations (11.27) into (11.25) and (11.26), and choosing the algebraic numbers A and B appropriately, we find that $\sum_{n=0}^{\infty} u_n (A + Bn) P_{\ell n}(x_0) z_0^n$ is an algebraic multiple of a Ramanujan-type series for $1/\pi$; in other words,

$$\sum_{n=0}^{\infty} u_n (A + Bn) P_{\ell n}(x_0) z_0^n = \frac{C}{\pi} \quad (11.28)$$

where A , B and C are algebraic numbers.

In practice, all the algebraic numbers involved are very cumbersome, so the computations are quite involved. Because any identity of the form (11.28) is uniquely determined by the choice of τ_0 and N , these two quantities serve as natural data for the identity. Below we provide brief computational details for some examples only; however we have done all the required computations for each of our illustrative identities.

11.5.1. Sun's identities. Here we show that all identities from groups IV and V in [183] can be routinely proven by the techniques we have developed.

We begin by differentiating the identities in Theorem 11.3. In each of (11.10) and (11.11), let $F(t)$ denote the respective ${}_2F_1$ hypergeometric function and $G(t) := t \, dF/dt$. Furthermore, let $\tilde{F}(t) = F(1-t^2)$ in (11.10) and $\tilde{F}(t) = F(1-t^3)$ in (11.11), as well as $\tilde{G}(t) = G(1-t^2)$ and $\tilde{G}(t) = G(1-t^3)$, respectively. Then, standard

partial differentiation techniques yield the derivatives

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} n P_{2n} \left(\frac{(X+Y)(1-XY)}{(X-Y)(1+XY)} \right) \left(\frac{X-Y}{1+XY} \right)^{2n} \\ &= \frac{1+XY}{2(1+X+Y-XY)(1-X-Y-XY)} (XY(1-XY)\tilde{F}(X)\tilde{F}(Y) \\ & \quad - Y^2(1+X^2)\tilde{F}(X)\tilde{G}(Y) - X^2(1+Y^2)\tilde{F}(Y)\tilde{G}(X)) \end{aligned} \quad (11.29)$$

and

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n(\frac{2}{3})_n}{n!^2} n P_{3n} \left(\frac{X+Y-2X^2Y^2}{(X-Y)\sqrt{1+4XY(X+Y)}} \right) \left(\frac{X-Y}{\sqrt{1+4XY(X+Y)}} \right)^{3n} \\ &= \frac{\sqrt{1+4XY(X+Y)}}{(1-X-Y-2XY)((1+2XY)^2+(1+X+Y)(X+Y-2XY))} \\ & \quad \times (2XY(X+Y-XY(X^2+Y^2))\tilde{F}(X)\tilde{F}(Y) \\ & \quad - Y^3(1+2X^2(3Y+X))\tilde{F}(X)\tilde{G}(Y) - X^3(1+2Y^2(3X+Y))\tilde{F}(Y)\tilde{G}(X)). \end{aligned} \quad (11.30)$$

(These can also be found without partial differentiation, since we can differentiate with respect to x and to z , then eliminate the P'_{2n} or P'_{3n} term.)

All group IV identities in [183] correspond to the form (11.10). The arguments of the hypergeometric functions on the right-hand side of (11.10) take the form $t(\tau_0)$ and $t(\tau_0/N)$ (or $1-t(\tau_0/N)$ in case (IV1)), where

$$\begin{aligned} \text{(IV1)} \quad \tau_0 &= \frac{i\sqrt{5/3}+1}{4}, \quad N=2; & \text{(IV2)} \quad \tau_0 &= \frac{3i\sqrt{5}+5}{4}, \quad N=5; & \text{and} \\ \text{(IV3)} \quad \tau_0 &= \frac{i\sqrt{85}+5}{4}, \quad N=5. \end{aligned}$$

It is further hypothesized in [183] that group IV contains all such series with rational parameters. Our analysis shows that the identities (IV5)–(IV18) all have τ_0 of the form $\sqrt{-pq/8}$ and $N=p$, where p and q are odd primes and the class number of the quadratic field $\mathbb{Q}(\tau_0)$ is 4. For the class number condition to be satisfied, p, q can only be taken from the seemingly exhaustive list $\{3, 5, 7, 13, 17, 19\}$. Thus our analysis lends weight to Sun's hypothesis.

Identity (V1) in [183] is of the form (11.11) and may be similarly analysed and proven. In this case we in fact have $t(3\tau_0) = t(15\tau_1)$, where $t(\tau_0) = \alpha$, $t(\tau_1) = \beta$ and $\tau_0 = (i\sqrt{91}+3)/6$.

The only remaining case, identity (IV4), is particularly pretty and lends itself as an example for our analysis. It states

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} \frac{8n+1}{6^n} P_{2n}\left(\frac{5}{2\sqrt{6}}\right) = \frac{10\sqrt{2}}{3\pi}. \quad (11.31)$$

The left-hand side corresponds to the choice $X = (4\sqrt{3} + 7)(5\sqrt{2} - 7)$, $Y = \sqrt{2} - 1$, $\tau_0 = 3i/(2\sqrt{2})$, and $N = 3$. So $\alpha = 1 - X^2$ and $\beta = 1 - Y^2$ in the notation of (11.25). Using the degree 3 modular equation and multiplier for $s = 1/2$, we deduce that

$$F(\alpha) = \frac{1 - \sqrt{2} + \sqrt{6}}{3} F(\beta),$$

$$G(\alpha) = \frac{172\sqrt{6} + 243\sqrt{3} - 298\sqrt{2} - 421}{3} F(\beta) + (235\sqrt{6} + 332\sqrt{3} - 407\sqrt{2} - 575)G(\beta).$$

With the help of (11.29) and the above relations, identity (IV4) is reduced to

$$\left(\frac{20}{3} - 5\sqrt{2}\right)F^2(\beta) + \left(20 - \frac{40\sqrt{2}}{3}\right)F(\beta)G(\beta) = \frac{10\sqrt{2}}{3\pi}.$$

Another computation relates $F(\beta)$ and $G(\beta)$ to $F(1-\beta)$ and $G(1-\beta)$ (the details can be found in Chapter 10), which enables us to apply Clausen's formula; (IV4) thus holds because Clausen's formula produces a form equivalent to the Ramanujan-type series [30, eqn. (4.1)]

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^3}{n!^3} (3 - 2\sqrt{2} + (8 - 5\sqrt{2})n)(2\sqrt{2} - 2)^{3n} = \frac{1}{\pi}.$$

The other cases can be done similarly but the algebra is formidable. For instance, in (IV7), using the notation of (11.10), we have

$$\left\{ \begin{array}{l} X \\ Y \end{array} \right\} = -171 \mp 120\sqrt{2} \pm 98\sqrt{3} \pm 76\sqrt{5} + 70\sqrt{6} + 54\sqrt{10} - 44\sqrt{15} \mp 31\sqrt{30}.$$

Remark 11.5.1. In Chapter 10 we produced “companion series” which involve derivatives of $P_n(x)$ in the summand. The series considered here also admit companion series; as an example, a companion to (IV4) is

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} \frac{1}{6^n} \left[P_{2n}\left(\frac{5}{2\sqrt{6}}\right) + 8\sqrt{6}n P_{2n-1}\left(\frac{5}{2\sqrt{6}}\right) \right] = \frac{14\sqrt{2}}{3\pi}.$$

◇

11.5.2. New series for $1/\pi$. Using (11.10) and the theory developed in Chapter 10 and outlined in the beginning of this section, we can produce series for $1/\pi$ at will. The following two are among the neatest:

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} (2 + 15n) P_{2n} \left(\frac{3\sqrt{3}}{5} \right) \left(\frac{2\sqrt{2}}{5} \right)^{2n} = \frac{15}{\pi}, \quad (11.32)$$

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} n P_{2n} \left(\frac{45}{17\sqrt{7}} \right) \left(\frac{4\sqrt{14}}{17} \right)^{2n} = \frac{68}{21\pi}. \quad (11.33)$$

For the first formula, $\tau_0 = i\sqrt{3}/2$ and $N = 3$, while for the second, $\tau_0 = i\sqrt{7}/2$ and $N = 7$. Note that as these are precisely the 3rd and 7th singular values of the complete elliptic integral K , we may prove each series directly without resorting to a Ramanujan-type series (which are, of course, closely tied with the theory of singular values, see Chapter 12). The second formula comes from the Ramanujan series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^3}{n!^3} \frac{5 + 42n}{64^n} = \frac{16}{\pi}. \quad (11.34)$$

To demonstrate that the choice of τ_0 is not confined to the singular values, here is another example corresponding to $\tau_0 = i\sqrt{3}/2$ and $N = 2$:

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} (5 - \sqrt{6} + 20n) P_{2n} \left(\frac{17}{15} \right) \left(\frac{217 - 88\sqrt{6}}{25} \right)^n = \frac{3(4 + \sqrt{6})}{2\pi}.$$

Similarly, in (11.11), we can take $\tau_0 = 2i/3$ and $N = 2$, therefore

$$\alpha = \frac{3(465 + 413\sqrt{3} - 3\sqrt{30254\sqrt{3} - 13176})}{5324} \quad \text{and} \quad \beta = \frac{3(3 - \sqrt{3})}{4}.$$

The algebraic numbers involved in (11.11) simplify remarkably, and aided by (11.30), we produce the new series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} (1 + 9n) P_{3n} \left(\frac{4}{\sqrt{10}} \right) \left(\frac{1}{\sqrt{10}} \right)^{3n} = \frac{\sqrt{15 + 10\sqrt{3}}}{\pi\sqrt{2}}, \quad (11.35)$$

whose truth is equivalent to the following series for $1/\pi$,

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{1}{2})_n (\frac{2}{3})_n}{n!^3} (1 + (5 + \sqrt{3})n) \left(\frac{3(7\sqrt{3} - 12)}{2} \right)^n = \frac{2 + \sqrt{3}}{\pi}.$$

Note that each term in the sums of (11.32), (11.33) and (11.35) is *rational*. More of Sun's conjectures are proven in Chapter 12.

11.5.3. New series for $1/\pi$ with Apéry-like sequences. As one of the consequences of Theorem 11.2, we exhibit here some new series of the form

$$\sum_{n=0}^{\infty} u_n(A + Bn)P_n(x_0)z_0^n = \frac{C}{\pi}, \quad (11.36)$$

where u_n satisfies (11.5). As such series are not the main goal of this chapter but rather curiosities, we will only list the relevant τ_0 , N and the final result.

We start with entry (a) of Table 1. Denoting the sequence by $u_n^{(a)}$ (and other entries in the table are denoted similarly), we have the generating function

$$\sum_{n=0}^{\infty} u_n^{(a)} x^n = \frac{1}{1-2x} {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \mid \frac{27x^2}{(1-2x)^3}\right).$$

Therefore, combined with Theorem 11.2, we can analyse (11.36) for $u_n^{(a)}$ as we did in Chapter 10. Indeed, taking $\tau_0 = 2i\sqrt{2/3}$ and $N = 2$, we have

$$\sum_{n=0}^{\infty} u_n^{(a)} (7 - 2\sqrt{3} + 18n) P_n\left(\frac{1 + \sqrt{3}}{\sqrt{6}}\right) \left(\frac{2 - \sqrt{3}}{2\sqrt{6}}\right)^n = \frac{27 + 11\sqrt{3}}{\pi\sqrt{2}}.$$

This is in fact equivalent to the classical series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{1}{2})_n (\frac{2}{3})_n}{n!^3} \frac{1 + 6n}{2^n} = \frac{3\sqrt{3}}{\pi}.$$

Next, for entry (b), there is no simple hypergeometric generating function (the sequence was used by Apéry to prove the irrationality of $\zeta(2)$). Nevertheless, using results from [71], we pick $\tau_0 = 2i\sqrt{2/5}$, $N = 2$, and obtain

$$\sum_{n=0}^{\infty} u_n^{(b)} (16 - 5\sqrt{10} + 60n) P_n\left(\frac{5\sqrt{2} + 17\sqrt{5}}{45}\right) \left(\frac{5\sqrt{2} - 3\sqrt{5}}{5}\right)^n = \frac{135\sqrt{2} + 81\sqrt{5}}{\pi\sqrt{2}}.$$

The generating function of $u_n^{(c)}$ is

$$\sum_{n=0}^{\infty} u_n^{(c)} x^n = \frac{1}{1+3x} {}_2F_1\left(\frac{1}{3}, \frac{2}{3} \mid \frac{27x(1-x)^2}{(1+3x)^3}\right).$$

The sequence gives $W_3(2n)$ in Chapter 1. Again, Theorem 11.2 applies; as an example, for $\tau_0 = i$, $N = 3$, and using the same $1/\pi$ series as for (11.35), we have

$$\sum_{n=0}^{\infty} u_n^{(c)} (7 - 3\sqrt{3} + 22n) P_n\left(\frac{\sqrt{14\sqrt{3} - 15}}{3}\right) \left(\frac{\sqrt{2\sqrt{3} - 3}}{9}\right)^n = \frac{9(9 + 4\sqrt{3})}{2\pi}.$$

For entry (d), we can take $\tau_0 = i\sqrt{3}/2$, $N = 3$, and produce the new series

$$\sum_{n=0}^{\infty} u_n^{(d)} (4 - 2\sqrt{6} + 15n) P_n \left(\frac{24 - \sqrt{6}}{15\sqrt{2}} \right) \left(\frac{4 - \sqrt{6}}{10\sqrt{3}} \right)^n = \frac{6(7 + 3\sqrt{6})}{\pi}.$$

For entry (f), we found after some searching that by using $\tau_0 = 1 + i\sqrt{7}/3$ and $N = 2$,

$$\sum_{n=0}^{\infty} u_n^{(f)} (7 - \sqrt{21} + 14n) P_n \left(\frac{\sqrt{21}}{5} \right) \left(\frac{7\sqrt{21} - 27}{90} \right)^n = \frac{5\sqrt{7}\sqrt{7\sqrt{21} + 27}}{4\pi\sqrt{2}}.$$

As for the last sporadic example (g), we take $\tau_0 = 2i/\sqrt{3}$ and $N = 2$ (i. e. the same data as (III) in Chapter 10) to generate the compact-looking series

$$\sum_{n=0}^{\infty} u_n^{(g)} n P_n \left(\frac{5}{3\sqrt{3}} \right) \left(\frac{1}{6\sqrt{3}} \right)^n = \frac{9\sqrt{3}}{2\pi}.$$

As stated earlier, the Legendrian entries are binomial transforms of the hypergeometric entries in Table 1, therefore the $1/\pi$ series for them are comparatively easy to find; we list one example for each entry below:

$$\begin{aligned} \sum_{n=0}^{\infty} u_n^{(e)} (8n - 1) P_n \left(\frac{26}{15\sqrt{3}} \right) \left(\frac{\sqrt{3}}{80} \right)^n &= \frac{15\sqrt{3}}{2\pi\sqrt{2}}, \\ \sum_{n=0}^{\infty} u_n^{(h)} (125n + 42) P_n \left(\frac{463}{182\sqrt{6}} \right) \left(-\frac{\sqrt{3}}{90\sqrt{2}} \right)^n &= \frac{546\sqrt{3}}{25\pi}, \\ \sum_{n=0}^{\infty} u_n^{(i)} (363n + 109) P_n \left(\frac{746}{425\sqrt{3}} \right) \left(-\frac{17}{2048\sqrt{3}} \right)^n &= \frac{7600\sqrt{2}}{33\pi\sqrt{11}}, \end{aligned}$$

and

$$\begin{aligned} \sum_{n=0}^{\infty} u_n^{(j)} \left(\frac{2n+1}{2457} - \frac{139}{4875\sqrt{17^3}} \right) P_n \left(\frac{2456}{2457} \right) \left(\frac{4081 - 57\sqrt{17^3}}{359424} \right)^n \\ = \frac{\sqrt{7}\sqrt{4081\sqrt{17} + 16473}}{17^3 \cdot 250\pi\sqrt{2}}. \end{aligned}$$

The corresponding data for the identities are as follows: $\tau_0 = i\sqrt{3}$, $N = 3$; $\tau_0 = i\sqrt{2}$, $N = 2$; $\tau_0 = i\sqrt{3}$, $N = 2$; and $\tau_0 = 1 + i\sqrt{7}$, $N = 2$, respectively.

11.6. Concluding remarks

We briefly outline the genesis of Theorems 11.1–11.3. While working on the project [74] (Chapter 10), it became clear that generating functions of type (11.10) and (11.11) should exist. Our confidence was boosted by examples like (11.31) in [183]. We learned, after coming across Theorem B, that generating functions

of $P_{\ell n}(x)$ could be obtained by generating functions of $P_n(x)$ multiplied by an arithmetic sequence. We then studied Brafman’s proof of Theorem A using Bailey’s identity (11.4), at which point it dawned on us that a more general form of the identity was needed to encompass not just hypergeometric, but arithmetic sequences. Inspired by the form of (11.13), we empirically discovered Theorem 11.1 which meets this goal and also contains (11.13) as a special case. Therefore, the significance of ‘arithmeticity’ has been a major driving force towards Theorem 11.3.

We expect that our Theorem 11.1 can be generalised even further to include the general form of Bailey’s transform [25, §9.6] and Clausen’s formula, both of which depend on more than one parameter. This could possibly imply new generating functions of Jacobi and other orthogonal polynomials. (Some experimental observations about orthogonal polynomials can also be found in Chapter 14.)

Our motivation for this chapter came from the remarkable work of Fred Brafman on generating functions of orthogonal polynomials. Before his untimely death at age 35, he solely authored ten mathematical papers, all about orthogonal polynomials; the works [63] and [64] are his first and last publications, respectively.

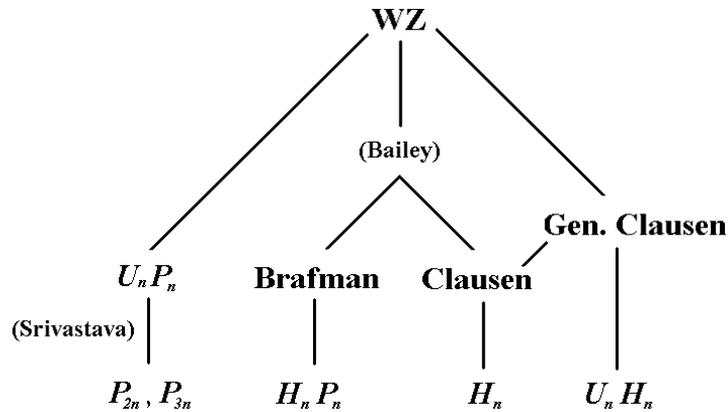


FIGURE 1. The relationships between various theorems used in producing series for $1/\pi$. Bold font indicates theorems (WZ stands for our main theorem 11.1); italic font indicates the types of coefficients in the series (U_n : Apéry-like sequence, P_n : Legendre polynomial, H_n : hypergeometric term); bracketed terms indicate theorems used but not directly involved in producing the series; downward lines indicate causal relationship, where the lower theorem can be derived from the higher one.

New Series for $1/\pi$

ABSTRACT. In this chapter, we outline a number of results relating to $1/\pi$ and other constants which do not fit the forms delineated in Chapters 10 and 11. We pay special attention to applications of Brafman's formula, and mention $1/\pi$ series which are contiguous to the classical ones. We then resolve some other conjectures of Sun. Finally, we describe a new method to generate $1/\pi$ series using Legendre's relation.

12.1. Orthogonal polynomials

12.1.1. Consequences of Brafman's and Srivastava's theorems. We recall Brafman's formula (10.4)

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} P_n(x) z^n = {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| \alpha\right) {}_2F_1\left(\begin{matrix} s, 1-s \\ 1 \end{matrix} \middle| \beta\right), \quad (12.1)$$

where $\alpha = (1 - \rho - z)/2$, $\beta = (1 - \rho + z)/2$, and $\rho = (1 - 2xz + z^2)^{1/2}$.

By putting $x = 0$ in Brafman's formula, we get the identity

$${}_4F_3\left(\begin{matrix} \frac{1-s}{2}, \frac{1+s}{2}, \frac{2-s}{2}, \frac{s}{2} \\ \frac{1}{2}, 1, 1 \end{matrix} \middle| -z^2\right) = F\left(\frac{1 - \sqrt{1 + z^2} - z}{2}\right) F\left(\frac{1 - \sqrt{1 + z^2} + z}{2}\right),$$

where F stands for the ${}_2F_1$. On the other hand, letting s be an integer in (12.1), we deduce the following non-obvious result:

$$\sum_{n=0}^k \frac{(-k)_n(k+1)_n}{n!^2} P_n\left(\frac{1-xy}{x-y}\right) \left(\frac{x-y}{2}\right)^n = P_k(x)P_k(y).$$

Note that $P_{-1/2}(1 - 2x^2) = 2/\pi K(x)$.

Since Brafman's formula is more general than the form (12.1) stated here – it in fact works for all Jacobi polynomials [63], we can apply it to other specialisations of Jacobi polynomials, e. g. the Chebyshev polynomials (encountered in Chapters

6 and 7). We can use it to deduce

$$\begin{aligned} \sum_{n=0}^{\infty} \binom{2n}{n} T_n(x) (z/4)^n &= \frac{\sqrt{1-xz+\rho}}{\sqrt{2\rho}}, \\ \sum_{n=0}^{\infty} \binom{2n}{n} U_n(x) (z/4)^n &= \frac{1+\rho}{\sqrt{2\rho}\sqrt{1-xz+\rho}}. \end{aligned} \tag{12.2}$$

Srivastava’s theorem (Theorem B, Chapter 11) is also very versatile for producing identities. Taking $N = 1$ in Srivastava’s theorem and the exponential generating function

$$\sum_{n=0}^{\infty} P_n(x) \frac{z^n}{n!} = e^{zx} J_0(z\sqrt{1-x^2}),$$

we deduce

$$\sum_{n=0}^{\infty} L_n(1) P_n(x) z^n = \frac{1}{\rho} \exp\left(\frac{z(z-x)}{\rho^2}\right) J_0\left(\frac{-z\sqrt{1-x^2}}{\rho^2}\right), \tag{12.3}$$

where L_n denotes the *Laguerre* polynomial.

Taking $N = 2$ and the sequence $(1 - 1/y^2)^k$ in Srivastava’s theorem, we obtain a connection with Chebyshev polynomials of the first kind (here $y' = \sqrt{1-y^2}$),

$$\begin{aligned} 2 \sum_{n=0}^{\infty} P_n(x) T_n(y) z^n & \tag{12.4} \\ = [1 - z(2(iy' - y)(yz - x) + z)]^{-\frac{1}{2}} & + [1 + z(2(iy' + y)(yz - x) - z)]^{-\frac{1}{2}}. \end{aligned}$$

Results like (12.2), (12.3), (12.4) and (12.7) may well find applications in harmonic analysis, though this has not been carefully investigated yet.

Remark 12.1.1. The ordinary generating function for P_n^2 is also a ${}_2F_1$,

$$\sum_{n=0}^{\infty} P_n(x)^2 z^n = \frac{1}{1-z} {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| \frac{4z(x^2-1)}{(1-z)^2}\right).$$

We may square both sides of the above formula in order to produce series for $1/\pi$, as outlined in Section 12.2. One example is

$$\sum_{n=0}^{\infty} \sum_{k=0}^n P_k(\sqrt{5})^2 16^k \binom{2n-2k}{n-k}^2 \left(\frac{17-12\sqrt{2}}{16}\right)^n (3\sqrt{2}-4+4\sqrt{2}n) = \frac{7+5\sqrt{2}}{2\pi}.$$

Another generating function, also given by Brafman, can in fact be easily verified using Srivastava’s theorem:

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n}{n!} P_n(x) z^n = \frac{1}{\sqrt{1-xz}} {}_2F_1\left(\frac{1}{4}, \frac{3}{4} \middle| \frac{z^2(x^2-1)}{(1-xz)^2}\right). \tag{12.5}$$

◇

12.1.2. Product of two Legendre polynomials. Our aim is to derive a generating function for the product of two *different* Legendre polynomials. We start with the representation

$$P_{2n}(x) = {}_2F_1\left(\begin{matrix} -n, n + \frac{1}{2} \\ 1 \end{matrix} \middle| 1 - x^2\right).$$

Substituting this into the sum below and interchanging the order of summation, we have

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n}{n!} P_{2n}(x) z^n = \frac{1}{\sqrt{1-z}} {}_2F_1\left(\begin{matrix} \frac{1}{4}, \frac{3}{4} \\ 1 \end{matrix} \middle| \frac{4z(x^2-1)}{(1-z)^2}\right), \tag{12.6}$$

compare with (12.5).

As pointed out by W. Zudilin, we can take $N = 2$ and $\lambda_k = (1/2)_k/k!$ in Srivastava’s theorem; the resulting sequence A_n essentially becomes the Legendre polynomials, so we have

$$\sum_{n=0}^{\infty} P_n(x)P_n(y)z^n = \sum_{n=0}^{\infty} \frac{(-1)^n (\frac{1}{2})_n}{\rho n!} P_{2n}\left(\frac{x-yz}{\rho}\right) \left(\frac{z\sqrt{1-y^2}}{\rho}\right)^{2n},$$

where $\rho = \sqrt{1-2xyz+y^2z^2}$. Simplifying the right hand side using (12.6), we obtain the desired generating function,

$$\sum_{n=0}^{\infty} P_n(x)P_n(y)z^n = (1-2xyz+z^2)^{-\frac{1}{2}} {}_2F_1\left(\begin{matrix} \frac{1}{4}, \frac{3}{4} \\ 1 \end{matrix} \middle| \frac{4(1-x^2)(1-y^2)z^2}{(1-2xyz+z^2)^2}\right). \tag{12.7}$$

Even though such a generating function was previously known (e.g. [146]), the above representation seems to be the most succinct one.

12.1.3. Series for another constant. Here we demonstrate a series for a related constant using Brafman’s formula. We start with the transformation for the *Jacobi polynomials* [2, Chapter 22]:

$$P_{2n}^{(a,a)}(x) = \frac{\Gamma(2n+a+1)n!}{\Gamma(n+a+1)(2n)!} P_n^{(a,-1/2)}(2x^2-1).$$

Take $a = 0$ above, we get $P_{2n}(x) = P_n^{(0,-1/2)}(2x^2-1)$. Now apply the general version of Brafman’s formula with $s = 1/4$ [63] to the right hand side. We obtain

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n^2}{(\frac{1}{2})_n n!} P_{2n}\left(\sqrt{\frac{x+1}{2}}\right) z^n = {}_2F_1\left(\begin{matrix} \frac{1}{4}, \frac{1}{4} \\ 1 \end{matrix} \middle| \frac{1-z-\rho}{2}\right) {}_2F_1\left(\begin{matrix} \frac{1}{4}, \frac{1}{4} \\ \frac{1}{2} \end{matrix} \middle| \frac{1+z-\rho}{2}\right).$$

The hypergeometric side simplifies in terms of $F := {}_2F_1(\frac{1}{2}, \frac{1}{2}; 1; x)$, and we produce the formula

$$\begin{aligned} \frac{2\sqrt{\pi}}{\Gamma(\frac{3}{4})^2} \sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n^2}{(\frac{1}{2})_n n!} P_{2n} \left(\sqrt{\frac{x+1}{2}} \right) z^n &= F \left(\frac{1 - \sqrt{(1+z+\rho)/2}}{2} \right) \\ &\times \left[F \left(\frac{1 - \sqrt{(1+z-\rho)/2}}{2} \right) + F \left(\frac{1 + \sqrt{(1+z-\rho)/2}}{2} \right) \right]. \end{aligned} \quad (12.8)$$

If we denote the argument of the first F by α and that of the second F by β , and choose them such that $\alpha = t(\tau)$, $\beta = t(\tau/N)$, then the right hand side of (12.8) equals

$$F(\alpha)(F(\beta) + F(1 - \beta)),$$

which, by the theory in Chapter 10, can be expressed in terms of $F(\alpha)^2$ alone; moreover, its z -derivative can be expressed in terms of $F(\alpha)^2$, $F(\alpha)G(\alpha)$, and $1/\pi$ alone. Hence, by taking a suitable linear combination, we get a series for $2\Gamma^2(3/4)/\pi^{3/2} = 1/K(1/\sqrt{2})$.

The calculations involved are formidable, so we only give one example: take $\tau = \sqrt{-3}$, $N = 3$, then

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n^2}{(\frac{1}{2})_n n!} (931 - 265\sqrt{6} + 6960n) P_{2n} \left(3\sqrt{\frac{5428793 - 2027520\sqrt{6}}{4113409}} \right) \\ \times (22154753 - 9044640\sqrt{6})^n = \frac{11128 + 4583\sqrt{6}}{16} \cdot \frac{\Gamma(\frac{3}{4})^2}{\pi^{3/2}}. \end{aligned}$$

12.2. Orr-type theorems and contiguous relations

In this section, we first supply some details on how to prove Ramanujan-type series [164], the existence and form of which are given in Proposition 10.5. The details, glossed over in previous chapters (except in Section 10.10, where a modular approach is presented), are based on the theory of singular values outlined in [46, Ch. 5]; this approach relies more on hypergeometric function theory and is more accessible than Section 10.10. Using the same theory, we also present some $1/\pi$ series that are *contiguous* to the ones studied by Ramanujan.

It is known that the singular values k_r , i. e. values such that $K'(k_r)/K(k_r) = \sqrt{r}$, are effectively computable algebraic numbers. It turns out that $E(k_r)$ is related to $K(k_r)$ via the equation [46, Ch. 5]

$$E(k_r) = \left(1 - \frac{\alpha_r}{\sqrt{r}}\right) K(k_r) + \frac{\pi}{4K(k_r)\sqrt{r}}, \quad (12.9)$$

where α_r denotes singular values of the *second kind*, which are again computable and algebraic. (In fact, for large r , α_r approaches $1/\pi$, and this serves as the basis for some fast iterations to compute π .)

The first step is to represent K^2 as a ${}_3F_2$ by Clausen’s formula, see (10.19) with $s = 1/2$. Next, we write out the ${}_3F_2$ as a sum and construct a linear combination of the sum with its t -derivative. We substitute $t = k_r$ and eliminate the $E(k_r)$ term with (12.9). Finally, we choose the coefficients in the linear combination so that all the $K(k_r)$ terms are also eliminated. Simple linear algebra shows that this can be done, and the result is the $1/\pi$ series

$$\frac{1}{\pi} = \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^3}{n!^3} (4k_r^2(1 - k_r^2))^n (\sqrt{r}(1 - 2k_r^2)n + \alpha_r - \sqrt{r}k_r^2). \tag{12.10}$$

Since it is readily verified by Euler’s transform (6.32) and the quadratic transform (6.4) that

$$\begin{aligned} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| 4x^2(1 - x^2)\right) &= \frac{1}{1 - x^2} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| \frac{-4x^2}{(1 - x^2)^2}\right) \\ &= \frac{1}{\sqrt{1 - x^2}} {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| \frac{-x^4}{4(1 - x^2)}\right), \end{aligned} \tag{12.11}$$

applying the above procedure to the two hypergeometric functions on the right, we obtain two more series:

$$\frac{1}{\pi} = \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^3}{n!^3} \left(\frac{-4k_r^2}{(1 - k_r^2)^2}\right)^n \left(\frac{\alpha_r}{1 - k_r^2} + \frac{1 + k_r^2}{1 - k_r^2} \sqrt{r} n\right), \tag{12.12}$$

$$\frac{1}{\pi} = \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^3}{n!^3} \left(\frac{-k_r^4}{4(1 - k_r^2)}\right)^n \frac{\alpha_r - \sqrt{r}k_r^2/2 + \sqrt{r}(2 - k_r^2)n}{\sqrt{1 - k_r^2}}. \tag{12.13}$$

These three series, using $r \in \{1, 2, 3, 4, 7\}$, give all four rational series for $1/\pi$ with $s = 1/2$: (12.19), (12.53), (12.67), and (11.34). By appropriate transformations such as (10.36) and (7.29), they also give $1/\pi$ series for other s . The transforms in (12.11) are not exhaustive, for instance, from

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| \frac{16x(1 - x)^2}{(1 + x)^4}\right) = \frac{4(1 + x)^2}{\pi} K(x)^2,$$

we can produce another series with argument $x(1 - x)^2/(4(1 + x)^4)$. We also repeat the remark from [46] that these ${}_3F_2$ ’s may be used to produce series for $K(k_r)$, by eliminating the $1/\pi$ term in the linear combination.

It is easy to see that, working along the same lines, one can deduce more formulas for $1/\pi$ as a linear combination of $F(z_0)$, $F'(z_0)$ and $F''(z_0)$ for some appropriate z_0 , as long as $F(z)$ is quadratic in K and E . (More generally, as long as $F(z)$ admits a modular parametrisation, bypassing the need to be hypergeometric, as seen for the Apéry-like sequence (b) in Chapter 11).

Example 12.2.1. As our first example, let $F(z) = K(z)^2$ (this is different from (12.10), where we used $F(4z^2(1-z^2)) = K(z)^2$). Taking a linear combination of the derivatives, applying (12.9), and choosing the coefficients to eliminate terms involving K , we obtain

$$\sum_{n=0}^{\infty} h(n) \left(\frac{k_r}{4}\right)^{2n} ((1-k_r^2)\sqrt{r}n + \alpha(r) - k_r^2\sqrt{r}) = \frac{1}{\pi}, \quad (12.14)$$

where $h(n)$ is defined in (6.26), and is a higher order Apéry-like analog to the sequence $\binom{2n}{n}^2$. When $r = 1$, we get

$$\sum_{n=0}^{\infty} \frac{nh(n)}{32^n} = \frac{2}{\pi}.$$

The paper [6] also investigates these series involving $h(n)$, and re-expresses everything in terms of k'_r . More general constructions involving higher order Apéry-like sequences are investigated in [71]. \diamond

More examples can come from two sources. Firstly, there are *Orr-type* theorems which allow us to write the product of two ${}_2F_1$'s as another hypergeometric function. Secondly, we can use contiguous relations: one hypergeometric function is *contiguous* to another if they have the same argument but their parameters differ by some integers (this is more closely looked at in Chapter 14). Both sources lead to the same type of $1/\pi$ series, with some extra rational function in the summand. Since the first approach uses published formulas, it is easier and we deal with it first.

Many Orr-type theorems are found in [26] and [179, §2.5]. For instance, a specialisation of [26, eqn. (7.4)] gives

$$(1-x)^2 {}_2F_1\left(\frac{1}{2}, \frac{1}{2} \middle| x\right) {}_2F_1\left(\frac{1}{2}, \frac{3}{2} \middle| x\right) = {}_3F_2\left(\frac{1}{2}, \frac{3}{2}, \frac{3}{2} \middle| \frac{-4x}{(1-x)^2}\right). \quad (12.15)$$

The left hand side of (12.15) can be easily written in terms of K and E :

$$\frac{\pi}{2} {}_2F_1\left(\begin{matrix} \frac{1}{2}, \frac{3}{2} \\ 1 \end{matrix} \middle| x^2\right) = \frac{E(x)}{1-x^2}, \quad \frac{\pi}{2} {}_2F_1\left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 2 \end{matrix} \middle| x^2\right) = \frac{2(E(x) - (1-x^2)K(x))}{x^2}.$$

Applying the procedure described above (i.e. taking a linear combination of the function and its derivative at singular values) allows us to produce series for $1/\pi$.

At the 2nd singular value, we have

$$\sum_{n=0}^{\infty} \binom{2n}{n}^3 \frac{(1+2n)^2(3+4n)}{1+n} \left(\frac{-1}{64}\right)^n = \frac{4}{\pi},$$

which is a contiguous version of (12.19), in the sense that their underlying ${}_3F_2$ parameters differ by some integers.

A different specialisation of [26, eqn. (7.4)] (with $\alpha = \beta = 3/4$, $\gamma = 2$) gives series with signature 4. The following fast converging rational series can be found by using the 37th singular value – it adds about 6 digits per term:

$$\begin{aligned} & \sum_{n=0}^{\infty} \binom{4n}{2n} \binom{2n}{n}^2 \frac{(1+2n)(1+4n)}{(1+n)^2} \left(\frac{-1}{14112^2}\right)^n \\ & \times (13977729825 + 27955478864n + 13977756400n^2) = \frac{3528^3}{\pi}. \end{aligned} \quad (12.16)$$

Many more series can be produced from results in [179]. Note however that [179, eqn. (2.5.27)] contains a misprint: $\frac{1}{2}c + \frac{1}{2}b - \frac{1}{2}$ should read $\frac{1}{2}c + \frac{1}{2}d - \frac{1}{2}$.

In the absence of Orr-type theorems, we can still express *any* function contiguous to $f(x) = {}_3F_2(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 1; x)$ in terms of K and E . This is because of Theorem 14.1, which states any such function is a linear combination of the derivatives of f , which are expressible with K and E (and the coefficients are functions of x). Therefore, we may find the left hand side of say (12.15) by applying the procedure in Chapter 14. Special cases of many Orr-type theorems boil down to contiguous relations, and therefore these special cases can be routinely proven. It also follows that any series contiguous to a rational series with rational argument are also rational.

Example 12.2.2. Here are a few of rational series found via the contiguous approach. Unlike the Ramanujan-type series which they originate from, typically n^2

terms (from the second derivative) are involved:

$$\begin{aligned} \sum_{n=0}^{\infty} \binom{2n}{n}^3 \frac{2n+1}{2n-1} \frac{n(6n-1)}{256^n} &= \frac{2}{\pi}, & \sum_{n=0}^{\infty} \binom{2n}{n}^3 \frac{(2n+1)^4}{n+1} \frac{1}{256^n} &= \frac{32}{3\pi}, \\ \sum_{n=0}^{\infty} \binom{2n}{n}^3 \frac{1-12n^2}{(1-2n)^2} \frac{1}{256^n} &= \frac{2}{\pi}, & \sum_{n=0}^{\infty} \binom{2n}{n}^3 \frac{6n+5}{(n+1)^2} \frac{1}{256^n} &= \frac{16}{\pi}, \\ \sum_{n=0}^{\infty} \binom{2n}{n}^2 \binom{4n}{2n} \frac{n(4n+1)(20n+1)}{(-1024)^n} &= \frac{-4}{\pi}. \end{aligned}$$

Their proofs are routine and proceed the same way as for (12.10); e.g. the first one comes from using the function

$$\frac{\pi^2}{4} {}_3F_2\left(\begin{matrix} -\frac{1}{2}, \frac{1}{2}, \frac{3}{2} \\ 1, 1 \end{matrix} \middle| 4x^2(1-x^2)\right) = (2E(x) - K(x))^2.$$

◇

12.3. A miscellany of results on π

12.3.1. Current status of Sun's conjectures. Sun's list of π conjectures have inspired much work in the field. For future reference, we list below all the proven or provable conjectures found in the the 24 Jan 2012 version (version 37) of [183]. The methods involved as also listed. By 'provable', we mean there is a general theory for proving the type of identity under question; even though the details can be formidable, they are still manageable given enough perseverance. A number of older entries, proven to Sun's satisfaction, appear underlined in [183].

- All of Conjecture I. [74] (Chapter 10)
- All of Conjecture II. [74]
- All of Conjecture III. [74]
- All of Conjecture IV. [193] (Chapter 11)
- A1 and A2. [74]
- Conjecture V. [193]
- Conjecture VII: 1, 3–6. [211]
- Conjecture 2: 1–3. [211]
- Conjecture 2: 4–9. Shown *here*, with ideas from [211]
- Conjecture 2: 10, 11. The sequence is Apéry-like, use [72]
- Conjecture 2: 12, 14, 20, 21. Shown *here*, ideas from [211]
- Conjecture 3: 11–19. [172]

- Conjecture 3: 11', 13', 15', 16', 18', 19', 20. Shown *here*, ideas from [211]
- Conjecture 4: 14. Same method as [6]
- Conjecture 5: 2–8. Shown *here*, ideas from [211]
- Conjecture 6: 1, 2. [211]

The main idea in [6] and [172] involves interchanging the order of summation. The latter paper provides rigorous details, and transforms some entries in conjecture 3 to entries in conjecture IV and their companion series, which have been proven in [193].

We remark that conjecture 4.14 can be routinely proven (it uses the same idea, i. e. interchange the order of summation, as [6]), and therefore all of Sun's Conjecture 4 is completely proven.

Conjectures 2.10 and 2.11 involve the sequence $S_k^{(2)}(4)$, which is just the Apéry-like sequence (e) in Chapter 11. Thus, they can be proven using the generating function

$$\sum_{n=0}^{\infty} \binom{2n}{n} u_n^{(e)} \left(\frac{x(1-32x+256x^2)}{(1-256x^2)^2} \right)^n = (1+16x) {}_2F_1 \left(\begin{matrix} \frac{1}{2}, \frac{1}{2} \\ 1 \end{matrix} \middle| 16x \right)^2.$$

With 2.10 we use $x = 1/32$; since the argument of the ${}_2F_1$ is $1/2$ in this case, the resulting $1/\pi$ series is particularly easy – see Section 10.8. With 2.11, we use $x = (4\sqrt{3} - 7)/16$, so after Euler's transformation (6.32), $16x/(16x - 1)$ becomes the 3rd singular value.

12.3.2. Hypergeometric evaluations. Many closed form evaluations for hypergeometric series are written as products of Gamma functions, for instance Gauss' theorem (5.3), and the partial list in Chapter 14. When the products of Gamma functions collapse to $1/\pi$, $1/\pi^2$, etc, we naturally obtain series for these constants. Such methods are explored in e. g. [76].

Example 12.3.1. Take the classical evaluation for a ${}_4F_3$ at -1 [11, Corollary 3.5.3], which is a consequence of Dougall's formula. Specialisations of the evaluation give equation (12.19) as well as

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{6}\right)_n^3}{n!^3} (-1)^n (1+12n) = \frac{3}{\pi}.$$

Clearly, many other Gamma evaluations may be found this way. Watson's formula (see Chapter 14) immediately gives

$$\sum_{n=0}^{\infty} \frac{1}{\binom{2n}{n}} \frac{4^n}{(2n+1)(n+2)(n+3)} = \frac{\pi^2}{32},$$

while Dougalls's formula gives

$$\sum_{k=0}^{\infty} \binom{2n}{n}^4 \frac{1}{2^{8n}} \frac{4n+1}{(n+1)(2n-1)} = \frac{-8}{\pi^2},$$

compare with (12.18) below. \diamond

Our next example, though still trivial, seems to be original. Take [98, eqn. (1.2)]; under the limit $n \rightarrow \infty$, we get

$${}_4F_3 \left(\begin{matrix} 2a, 2b, 1-2b, 1+2a/3 \\ a-b+1, a+b+1/2, 2a/3 \end{matrix} \middle| -\frac{1}{8} \right) = \frac{4^a \Gamma(1+a-b) \Gamma(1/2+a+b)}{\sqrt{\pi} \Gamma(1+2a)}. \quad (12.17)$$

For instance, with $a = b = 1/4$, we recover the series (12.67).

12.3.3. Fourier-Legendre expansion. Certain series for $1/\pi$ and other constants may be arrived at using the *Fourier-Legendre* expansion of a function. To be more precise, under mild conditions we can expand a function f in terms of the Legendre polynomials:

$$f(x) = \sum_{n=0}^{\infty} a_n P_n(x), \quad \text{where } a_n = \frac{2n+1}{2} \int_{-1}^1 P_n(x) f(x) dx.$$

For $f(x) = \sqrt{1-x^2}$, we can evaluate a_n by writing $P_n(x)$ as a sum and interchanging the order of integration and summation. After evaluating the sum by Dixon's theorem (14.14), we get

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{n!^2} \frac{4n+1}{(n+1)(1-2n)} P_{2n}(x) = \frac{4\sqrt{1-x^2}}{\pi}.$$

Setting $x = 0$ and using the evaluation for $P_n(0)$, this gives the series

$$\sum_{n=0}^{\infty} \binom{2n}{n}^3 \left(\frac{-1}{64}\right)^n \frac{4n+1}{(n+1)(1-2n)} = \frac{4}{\pi}.$$

Parseval's theorem applied to the same f produces a series for $1/\pi^2$,

$$\sum_{n=0}^{\infty} \binom{2n}{n}^4 \frac{1}{2^{8n}} \frac{4n+1}{(n+1)^2(2n-1)^2} = \frac{32}{3\pi^2}, \quad (12.18)$$

which is in fact contiguous to one of Guillera's many formulas [107, eqn. (14)].

Of course, we may use more general functions, for instance choose $f(x) = (1 - x^2)^{p-1/2}$. The $p = 0$ case recovers the first ever Ramanujan-type series for $1/\pi$, due to Bauer:

$$\sum_{n=0}^{\infty} \binom{2n}{n}^3 \left(\frac{-1}{64}\right)^n (4n + 1) = \frac{2}{\pi}. \tag{12.19}$$

The corresponding series for $1/\pi^2$ (explored over a century ago by Glaisher [99]) are all in fact hypergeometric evaluations using Dougall’s ${}_5F_4$ formula [11, Corollary 3.5.2].

12.3.4. Fourth powers of binomial coefficients. In this section we look at the generating function of the sums of fourth powers of binomial coefficients, and relate it to series for $1/\pi$.

Theorem 12.1. *In the neighbourhood of $x = 0$, let $u = u(x) = \sqrt{1 + 4x}$, $v = v(x) = \sqrt{1 - 16x}$. Then*

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 x^n = \frac{5}{3u + 2v} {}_3F_2\left(\begin{matrix} \frac{1}{4}, \frac{1}{2}, \frac{3}{4} \\ 1, 1 \end{matrix} \middle| \frac{4(u - v)^5(u + v)}{5(3u + 2v)^4}\right), \tag{12.20}$$

moreover, (12.20) can be used to produce series for $1/\pi$.

PROOF. Let $a(n) = \sum_{k=0}^n \binom{n}{k}^4$. Zeilberger’s algorithm is able to produce the recursion

$$n^3 a(n) = 2(2n - 1)(3n^2 - 3n + 1)a(n - 1) + (4n - 3)(4n - 4)(4n - 5)a(n - 2),$$

which can be routinely translated into a differential equation satisfied by the left hand side of (12.20), for instance using the *Maple* command `rectodiffeq`. It is also routine (though tedious) to check that the right hand side is annihilated by the same differential equation, and that the first few terms of the series expansion for both sides agree. Thus (12.20) holds.

Because the right hand side of (12.20) has the requisite ${}_3F_2$ form with signature 4, therefore by Proposition 10.5, at some computable x ’s there exists a linear combination of (12.20) and its derivative which evaluates to $1/\pi$. Alternatively, we may use the transformation

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

and appeal to the construction outlined in Section 12.2 (this is the approach we take subsequently). □

Example 12.3.2. On top of Yang's original example (5.8) which we reproduce below, the following $1/\pi$ series may be produced; they correspond to the 30th, 70th, 130th and 190th singular values of K respectively:

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 \frac{4n+1}{36^n} = \frac{18}{\sqrt{15}\pi}, \quad (12.21)$$

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 \frac{11+60n}{196^n} = \frac{98}{\sqrt{7}\pi}, \quad (12.22)$$

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 \frac{18+130n}{1296^n} = \frac{81}{\sqrt{2}\pi}, \quad (12.23)$$

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 \frac{47+408n}{5776^n} = \frac{1444}{\sqrt{95}\pi}. \quad (12.24)$$

The next three rational series have negative arguments, which essentially come from applying the transformation (12.11); they correspond to the 25th, 45th and 85th singular values of K :

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 \frac{1+3n}{(-20)^n} = \frac{5}{2\pi}, \quad (12.25)$$

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 \frac{1+4n}{(-64)^n} = \frac{32}{3\sqrt{15}\pi}, \quad (12.26)$$

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 \frac{3+17n}{(-324)^n} = \frac{81}{4\sqrt{5}\pi}. \quad (12.27)$$

We can produce many more (non-rational) series, for instance

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 (14 + 3(20 \mp \sqrt{15})n) \left(\frac{5\sqrt{10} \pm 3\sqrt{6}}{98} \right)^{2n} = \frac{2(78\sqrt{3} \pm 17\sqrt{5})}{(3 \mp 1)\pi}$$

comes from the 15th singular value. \diamond

Some entries in [183] are in fact related to the sum of fourth powers of binomial coefficients. The first connection is the following representation,

$$\sum_{k=0}^n \binom{2(n-k)}{n-k} \binom{n+k}{2k} \binom{n-k}{k} \binom{2k}{k} = \sum_{k=0}^n \binom{n}{k}^4. \quad (12.28)$$

This is easily proven using Zeilberger's algorithm (which is able to show that both sides satisfy the same recursion). From this, we get

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{2n}{n} \binom{n+2k}{2k} \binom{n}{k} \binom{2k}{k} x^{k+n} = \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 x^n. \quad (12.29)$$

Seven of Sun’s series in conjecture 5 [183] have the left hand side of (12.29) as a building block. It turns out that they correspond to the labeled equations in Example 12.3.2. We return to their proof in the next section.

The other connection comes from examining seven of the entries in conjecture 3 of [183]. For these entries, the argument in g_k and the square root of the geometric term differ by 2. It follows that these conjectural series for $1/\pi$ have the building block

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

More specifically, we need a linear combination of the above sum, and a similar one with an extra factor of n in the summand. The proof for those series involves ‘satellite identities’ which we describe in the next section. In particular, we will prove the key formula

Theorem 12.2. *In a neighbourhood of $x = 0$,*

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{2n}{n} \binom{n}{k}^2 \binom{2k}{k} \frac{x^{2n-k}}{(2x+1)^{2n+1}} = \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k}^4 x^n. \tag{12.30}$$

Equation (12.30) will show that these seven entries again correspond to the labeled equations in Example 12.3.2. It will be obvious that we may produce many more series of the same type. We remark that the inner summand on the left side of (12.30) is the Apéry-like sequence (c), which is $W_3(2k)$ in Chapter 1.

12.4. New generating functions

In this section we prove some more of Sun’s conjectures for $1/\pi$. The main ideas are taken from [211].

12.4.1. Satellite identity. Whenever we have a sum of the type

$$H = \sum_n h_n(x, z) = F(\alpha)F(\beta),$$

where H, α, β are functions of x and z , and additionally α and β are related by a modular equation of degree N , then for certain values of x and z , there always exists a non-trivial linear combination of H, H_x, H_z that is 0. The reason for this has already been explicated in Chapter 11, but we recapitulate it here. Suppose that x and z are chosen so that $\alpha = t(\tau_0)$ and $\beta = t(\tau_0/N)$, where t is a modular function and τ_0 is a quadratic irrationality. The modular equation allows us to write H in

terms of $F(\alpha)^2$. Also, the two derivatives of H each equals a linear combination of $F(\alpha)^2$ and $F(\alpha)G(\alpha)$, where $G(t) = t dF(t)/dt$. Thus we can always take a linear combination of these three terms to get 0.

Indeed, whenever N is fixed, this linear combination ends up being a functional equation of the form $\sum_n \tilde{h}_n(p) \equiv 0$, where we parametrise the left hand side by a single variable p . Producing such a functional equation algebraically is *easier* than finding a series for $1/\pi$; moreover, it can often be guessed and then proven using the Wilf-Zeilberger machinery. Functional equations of this type were first investigated in [211], where they are called *satellite identities*, since they play a secondary role in producing $1/\pi$ series as we shall see.

Example 12.4.1. We give some examples of satellite identities. In Theorem 11.3, take $N = 3$, we have the very succinct identity

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{n!^2} (4(p^2 - 1))^n ((3n + 1)P_{2n}(p) - p(2n + 1)P_{2n+1}(p)) = 0. \tag{12.31}$$

This can be proven using the degree 3 modular equation; alternatively, we can use the Wilf-Zeilberger algorithm to find a differential equation satisfied by the left hand side, but this approach involves more work.

Returning to Brafman’s formula (12.1), the degree 3 modular equation produces, for $s = 1/2$,

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{n!^2} (4p(1 - p^2))^n \left[\left(p + \left(2p - \frac{1}{2p} \right) n \right) P_n \left(\frac{1 + p^2}{2p} \right) - (n + 1) P_{n+1} \left(\frac{1 + p^2}{2p} \right) \right] = 0.$$

For $s = 1/3$ and $N = 2$, we have

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{3}\right)_n \left(\frac{2}{3}\right)_n}{n!^2} \left(\frac{27(p^2 - 1)}{4p^3} \right)^n \left[\left(\frac{1}{p} + n \left(\frac{3}{p} - \frac{4p}{3} \right) \right) P_n(p) - (n + 1) P_{n+1}(p) \right] = 0,$$

where we have used the parametrisation of the degree 2 modular equation in signature 3, and the recursion (14.25) satisfied by the Legendre polynomials. \diamond

12.4.2. A key observation. Many of Sun’s conjectures [183] involve sums of the form

$$\sum_{n=0}^{\infty} \sum_{k=0}^n F(n, k) x^k z^n,$$

where F is a hypergeometric term often expressible as the product of binomial coefficients. It is thus possible to find a differential equation in z for the double

sum. However, such differential equations often have degrees 4 or higher, making them not amenable for reduction in terms of hypergeometric functions. A key observation from [211] is that, in many (but not all) of Sun’s conjectures, x and z are often related by a simple *algebraic relation*. When this happens the corresponding differential equation often reduces to degree 3. This makes them much easier to solve, and in some instances *Maple* can give the solutions. Combined with satellite identities, [211] resolves several of Sun’s conjectures.

Remark 12.4.1. How can we discover such an algebraic relation between x and z ? Based on Sun’s numerical data, we have good reasons to suspect that potential algebraic relations transform the sums into

$$\sum_{n=0}^{\infty} \sum_{k=0}^n F(n, k) \frac{x^{k+n}}{(a + bx)^{2n+1}}, \text{ or } \sum_{n=0}^{\infty} \sum_{k=0}^n F(n, k) \frac{(-1)^n x^{k+n}}{(a + bx)^{n+1/2}}, \tag{12.32}$$

where a and b are to be determined. For general a and b , we compute sufficiently many terms of the x -expansion of (12.32) and check if they satisfy a three-term recurrence (corresponding to a degree 3 differential equation for the sum) with polynomial coefficients, where the degrees of the polynomials can be first specified. In terms of linear algebra, this comes down to checking if a certain determinant is zero for some a and b . The task of finding suitable integer values a and b in (12.32) (if they exist) can thus be accomplished by finding integer solutions to the determinant, which is a (complicated) polynomial expression in a and b .

Indeed, (12.29) was first discovered this way. ◇

Using either Sun’s data or the above procedure, we discover:

Theorem 12.3. *In a neighbourhood of $x = 0$,*

$$\begin{aligned} & \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} \binom{2n-2k}{n-k} \binom{2k}{k} \binom{2n}{n} \frac{x^{k+n}}{(1+4x)^{2n+1}} \\ &= \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} \binom{2n-2k}{n-k} \binom{2k}{k} \binom{2n}{n} \frac{(-1)^n x^{k+n}}{(1-8x)^{n+1/2}} = {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| 64x^2\right). \end{aligned} \tag{12.33}$$

PROOF. For each sum on the left hand side, write the coefficient of x as a double sum. We apply the multiple WZ algorithm to obtain a recursion for the coefficients; this step takes some time and produces a degree 9 recursion. Then, we simply show that the right hand side coefficients satisfy the same recursion and initial conditions.

Without the luxury of knowing the right hand side of (12.33), we can convert the recursion into a differential equation satisfied by the generating function and factorise it (using the `DFactor` command in *Maple*). This gives a 3rd order differential equation, which is solvable by *Maple* and can be rearranged into the right hand side of (12.33). \square

The satellite identities of (12.33) are given by

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} \binom{2n-2k}{n-k} \binom{2k}{k} \binom{2n}{n} \frac{x^{k+n}}{(1+4x)^{2n}} \left[1 + 3\left(1 + \frac{1}{4x}\right)k + \left(1 - \frac{1}{4x}\right)n \right] = 0,$$

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} \binom{2n-2k}{n-k} \binom{2k}{k} \binom{2n}{n} \frac{(-1)^n x^{k+n}}{(1-8x)^n} \left[4 + 3\left(1 - \frac{3}{x}\right)k + \left(8 + \frac{1}{x}\right)n \right] = 0.$$

To produce say the first one, we first managed to guess it. More precisely, for a small, irrational x we compute $a_0 = \sum_{n,k} A(n,k,x)$, $a_1 = \sum_{n,k} A(n,k,x)k$, and $a_2 = \sum_{n,k} A(n,k,x)n$, then asked PSLQ to find a null linear combination with integer coefficients among the elements of

$$\{a_0, a_1, a_2, a_0x, a_1x, a_2x, a_0x^2, a_1x^2, a_2x^2, \dots\}.$$

Once found, the satellite identity can be proven by extracting the coefficients of x , which is shown (in this case) to satisfy a 7th order recursion by the multiple WZ algorithm.

Note that the right hand side of (12.33) is a building block for $1/\pi$ series. We can differentiate both sides of (12.33), and take an appropriate linear combination to give $1/\pi$, as guaranteed by Proposition 10.5. However, the resulting series would involve linear terms in k coming from the derivative of (12.33). This is where the satellite identity comes in: we use it to eliminate the k term.

This way, Theorem 12.3 allows us to prove all of Sun’s conjectures involving $S_k^{(1)}$ (conjectures 2.4–2.9) [183], using only the 3rd and 7th singular values. An example of a series so proven is Sun’s entry 2.4,

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} \binom{2n-2k}{n-k} \binom{2k}{k} \binom{2n}{n} \frac{140n+19}{2^{6k}} \left(\frac{2}{17}\right)^{2n} = \frac{289}{3\pi}. \tag{12.34}$$

The coefficients in this type of series can be considered as extensions of the Apéry-like sequence (d). We can produce arbitrarily more $1/\pi$ series of the same type. For

instance, using the 4th singular value, we have the *complex series*

$$\begin{aligned} & \sum_{n=0}^{\infty} \sum_{k=0}^n \binom{n}{k} \binom{2n-2k}{n-k} \binom{2k}{k} \binom{2n}{n} \left(\frac{\sqrt{-2}}{32}\right)^k \left(\frac{16+31\sqrt{-2}}{1089}\right)^n (35-8\sqrt{-2}+132n) \\ &= \frac{116\sqrt{2}+95i}{2\pi}. \end{aligned} \tag{12.35}$$

Example 12.4.2. We return to (12.30). It is true simply because the multiple WZ algorithm can produce a recursion for the coefficients of x in the left hand side (albeit being order 6), which is also satisfied by the right hand side, and both sides agree to sufficiently many terms. Therefore, a linear combination of the left hand side and its derivative produces series for $1/\pi$. However, the derivative also involves a linear term dependent on k ; this term can be canceled out because of the satellite identity (first guessed by PSLQ, then proven by the multiple WZ algorithm):

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{2n}{n} \binom{n}{k}^2 \binom{2k}{k} \frac{x^{2n-k}}{(2x+1)^{2n}} \left[\frac{2}{x} + 1 - 2\left(\frac{1}{x} + 2\right) \left(\frac{1}{x} - 1\right)k + \frac{3}{2x} \left(\frac{1}{x} + 4\right)n \right] = 0.$$

Similarly, the satellite for (12.29) is

$$\sum_{n=0}^{\infty} \sum_{n=0}^k \binom{2n}{n} \binom{n+2k}{2k} \binom{n}{k} \binom{2k}{k} x^{k+n} [4x + 3(4x+1)k + 2(x-1)n] = 0.$$

As mentioned earlier, entries 11', 13', 15', 16', 18', 19', 20 from Sun's conjecture 3 [183] can be proven using (12.30), while entires 2–8 from conjecture 5 can be proven using (12.29); they are both equivalent to the series in Example 12.3.2. We give one example from each type of proven series:

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{2n}{n} \binom{n}{k}^2 \binom{2k}{k} \frac{14^{2k}}{198^{2n}} (3920n + 541) = \frac{42471}{8\sqrt{7}\pi}, \tag{12.36}$$

$$\sum_{n=0}^{\infty} \sum_{n=0}^k \binom{2n}{n} \binom{n+2k}{2k} \binom{n}{k} \binom{2k}{k} \frac{3245n + 268}{1296^{n+k}} = \frac{1215}{\sqrt{2}\pi}. \tag{12.37}$$

Finally, we note that [183] states that entries 3.11'–3.19' are equivalent to 3.11–3.19, and some of the latter entries have been proven in [172], though our analysis is computationally simpler. ◇

Entries in Sun's conjecture 2 [183] which involve $S_k^{(2)}$ generalise the Apéry-like sequence (e) (since $S_k^{(2)}(4)$ is (e) itself). When $z = 1/(x+4)^2$, as is the case for the four entries listed below, the resulting differential equation (again found by multiple WZ) can be solved by *Maple* in terms of the Heun G function (see [32, vol. 3]), with

the first parameter equal to 4. Using of [140, eqn. (3.5b)], this Heun G function reduces to the form ${}_2F_1(\frac{1}{6}, \frac{1}{3}; \frac{1}{2}; t(x))$. Applying Goursat's quadratic transform [103, p. 118, eqn. (25)], we finally discover

Theorem 12.4. *In a neighbourhood of $x = 0$,*

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{2n-2k}{n-k} \binom{2k}{k}^2 \binom{2n}{n} \frac{x^{k+n}}{(1+4x)^{2n+1}} = {}_3F_2\left(\begin{matrix} \frac{1}{3}, \frac{1}{2}, \frac{2}{3} \\ 1, 1 \end{matrix} \middle| 108x^2(1-4x)\right). \quad (12.38)$$

Its satellite identity is:

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{2n-2k}{n-k} \binom{2k}{k}^2 \binom{2n}{n} \frac{x^{k+n}}{(1+4x)^{2n}} \left[1 + 2k + n + \frac{2k-n}{4x}\right] = 0.$$

It follows that Sun's conjectures 2.12, 2.14, 2.20 and 2.21 can be proven. For the first one, the argument of the ${}_3F_2$ in (12.38) is 1 and so its proof follows by hypergeometric evaluations. The next three have arguments $1/2$, $2/27$ and $4/125$ respectively, equivalent to the (only) rational Ramanujan-type series for signature 3. As an example, entry 2.20 is

$$\sum_{n=0}^{\infty} \sum_{k=0}^n \binom{2n-2k}{n-k} \binom{2k}{k}^2 \binom{2n}{n} \frac{12n+1}{6^{2k}} \left(\frac{3}{20}\right)^{2n} = \frac{75}{8\pi}. \quad (12.39)$$

12.5. Series for $1/\pi$ using Legendre's relation

As stated in Proposition 10.5, Ramanujan-type series for $1/\pi$ originally took the form

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n (s)_n (1-s)_n}{n!^3} (a+bn) z_0^n = \frac{c}{\pi}, \quad (12.40)$$

where $s \in \{1/2, 1/3, 1/4, 1/6\}$. As we saw in Chapters 10 and 11, a more encompassing series for $1/\pi$ would look like

$$\sum_{n=0}^{\infty} U(n) p(n) z_0^n = \frac{c}{\pi^k}, \quad (12.41)$$

where $U(n)$ is an arithmetic sequence, and $p(n)$ is a polynomial (often linear or quadratic in n).

Most of the current methods for producing such series rely on one of the following methods:

- Hypergeometric series (Clausen's formula and singular values of K), see [46] and Section 12.2;

- Modular equations together with the first approach, see Chapters 10 and 11;
- Experimental mathematics (creative telescoping), explored in say [106];
- Summation formulas for hypergeometric series, Fourier-Legendre series, etc, see Section 12.3.

A notable feature of $1/\pi$ series produced using the methods above has been severe restrictions in the argument of the geometric term (z_0 in (12.41)), as z_0 may need to come from singular values of K , or be a special value for a summation formula to work. Here we give a new method for producing series for $1/\pi$, as well as some related constants, using only Legendre's relation. The method presented here breaks such restrictions so the argument can be any real number for which the underlying series converges.

12.5.1. Legendre's relation. Our analysis hinges on Legendre's relation [46, Theorem 1.6], which states

$$E(x)K'(x) + E'(x)K(x) - K(x)K'(x) = \frac{\pi}{2}. \quad (12.42)$$

We have already encountered Legendre's relation in Chapters 5 and 6. A more general form of (12.42) holds [46, equation (5.5.6)]:

$$E^s(x)K^{s'}(x) + E^{s'}(x)K^s(x) - K^s(x)K^{s'}(x) = \frac{\pi \cos(\pi s)}{2(1+2s)}, \quad (12.43)$$

where K^s , E^s are defined in (5.1) and (5.2). Note also that in (12.43), s is not restricted to the four values as in (12.40).

Suppose we have a factorisation of the following type:

$$\pi^2 G(z) = K(a(z))K(b(z)), \quad (12.44)$$

where G is analytic near the origin and satisfies an ordinary differential equation of degree no less than 4 – for instance, G could be a ${}_4F_3$. (The condition on the degree of the differential equation for G is imposed because we will solve a system of four equations below, so having three linearly independent derivatives help.) Suppose further that we can find a number z_0 such that $a(z_0)^2 = 1 - b(z_0)^2$, so that the right hand side of (12.44) becomes $K(a(z_0))K'(a(z_0))$. We then consider a linear

combination of derivatives of equation (12.44), namely

$$\begin{aligned} & \pi^2 \left(A_0 G(z_0) + A_1 \frac{d}{dz} G(z_0) + A_2 \frac{d}{dz^2} G(z_0) + A_3 \frac{d}{dz^3} G(z_0) \right) \\ & = B_0 K K'(z_0) + B_1 E K'(z_0) + B_2 E' K(z_0) + B_3 E E'(z_0), \end{aligned} \quad (12.45)$$

where A_i are constants that may depend on z_0 , while B_i depend on A_i . The equality in (12.45) holds because derivatives of E and K are again expressible in terms of E and K . It remains to solve (if possible) the following system of equations for A_i ,

$$B_0 = -1, \quad B_1 = 1, \quad B_2 = 1, \quad B_3 = 0,$$

so that we may apply Legendre's relation (12.42) to (12.45) and obtain, for those choices of A_i ,

$$A_0 G(z_0) + A_1 \frac{d}{dz} G(z_0) + A_2 \frac{d}{dz^2} G(z_0) + A_3 \frac{d}{dz^3} G(z_0) = \frac{1}{2\pi}. \quad (12.46)$$

A series for $1/\pi$ is thus obtained; when written as a sum, the left hand side typically contains a cubic of the summation variable. We will illustrate such series using different choices of G below.

12.5.2. Brafman's formula. An example of a factorisation in the form of (12.44) comes from Brafman's formula (12.1). Although the formula is of type (12.44), solving for $\alpha^2 = 1 - \beta^2$ only results in a trivial identity. Therefore our strategy is to modify the arguments α or β via some transformations.

12.5.2.1. *The $s = 1/2$ case.* Using $s = 1/2$ and applying the quadratic transform (6.5) to one of the terms in (12.1), we obtain

$$\frac{\pi^2}{4} \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{n!^2} P_n(x) z^n = \frac{1}{1 + \alpha^{1/2}} K\left(\frac{2\alpha^{1/4}}{1 + \alpha^{1/2}}\right) K(\beta^{1/2}). \quad (12.47)$$

This fits the type of (12.44). After significant amount of algebra as outlined by the approaches leading to (12.46), we have the following:

Theorem 12.5. For $k \in (0, 1)$,

$$\begin{aligned} & \sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{-k^4 + 6k^3 - 2k + 1}{(k^2 + 1)(k^2 + 2k - 1)}\right) \left(\frac{(k^2 + 1)(k^2 + 2k - 1)}{16(k + 1)^2}\right)^n (C_3 n^3 + C_2 n^2 + C_1 n + C_0) \\ & = \frac{2(k + 1)^3 (k^2 + 1)}{\pi}, \end{aligned} \quad (12.48)$$

where

$$\begin{aligned} C_3 &= 4(k-1)^2 k^2 (k^2 + 3k + 4)^2, \\ C_2 &= 12(k-1)k(k^6 + 5k^5 + 10k^4 + 10k^3 + 5k^2 - 3k + 4), \\ C_1 &= 9k^8 + 36k^7 + 37k^6 + 8k^5 - 9k^4 - 56k^3 + 63k^2 - 28k + 4, \\ C_0 &= (k^2 + 2k - 1)^2 (2k^4 + 3k^2 - 2k + 1). \end{aligned}$$

PROOF. A little algebra shows that if we choose

$$x = \frac{1 - 2k + 6k^3 - k^4}{(k^2 + 1)(k^2 + 2k - 1)}, \quad z_0 = \frac{(k^2 + 1)(k^2 + 2k - 1)}{(k + 1)^2},$$

then, viewing α and β as functions of z , we get $\beta(z_0)^{1/2} = k$, and $2\alpha(z_0)^{1/4}/(1 + \alpha(z_0)^{1/2}) = \sqrt{1 - k^2}$, as desired. With these choices we have $\alpha(z_0) = (1 - k)^2/(1 + k)^2$; we can also compute and simplify the derivatives $a'(z), a''(z), a'''(z)$ and $b'(z), b''(z), b'''(z)$ at $z = z_0$. Thus, as in (12.44), we have an equation of the type

$$\pi^2 \left[\frac{1 + \alpha(z)^{1/2}}{4} \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^2}{n!^2} P_n(x) z^n \right] = K \left(\frac{2\alpha(z)^{1/4}}{1 + \alpha(z)^{1/2}} \right) K(\beta(z)^{1/2}),$$

where at $z = z_0$ the arguments of the two K 's are complementary.

We take a linear combination (with coefficients A_i) of the z -derivatives of the above equation, as done in (12.45), then substitute in $z = z_0$ and simplify the resulting expression using the precomputed values for $\alpha'(z_0), \beta'(z_0)$ etc. Finally, we solve for A_i so that Legendre's relation may be applied to obtain a series of the form (12.46). The result, after tidying up, is (12.48).

We now look at the convergence. From the standard asymptotics for the Legendre polynomials [184], we have, as $n \rightarrow \infty$,

$$P_n(x) = O(|x + \sqrt{x^2 - 1}|^n) \text{ for } |x| > 1 \text{ and } P_n(x) = O(n^{-1/2}) \text{ for } |x| \leq 1.$$

Therefore, for any rational $k \in (0, 1)$, the sum in (12.48) converges geometrically, where the rate is given by

$$\frac{1 - 2k + 6k^3 - k^4}{(1 + k)^2} + 4 \left(\frac{k(1 - k)}{1 + k} \right)^{3/2}.$$

□

Note that any rational choice of $k \in (0, 1)$ leads to a *rational* series in Theorem 12.5, which is indicative that such series are likely to be fundamentally different from ones that are entirely modular in nature (see e. g. Chapter 10), whose arguments

are much more restricted. For instance, with the choice of $k = 1/2$ in Theorem 12.5, we get

$$\sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{11}{5}\right) \left(\frac{5}{576}\right)^n (14 - 171n - 4452n^2 + 2116n^3) = \frac{2160}{\pi}.$$

Theorem 12.5 is by no means the unique consequence of (12.1) with $s = 1/2$. For example, we can apply quadratic transformations to both arguments on the right hand side of (12.1). The result is also a rational series, convergent for $k \in (0, 1)$ and genuinely different from Theorem 12.5, though the general formula is too messy to be exhibited here. We give only one instance (with the choice $k = 1/2$) here:

$$\begin{aligned} \sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{19}{13}\right) \left(\frac{65}{20736}\right)^n (97756868n^3 - 24254580n^2 - 539415n - 264590) \\ = \frac{6065280}{\pi}. \end{aligned}$$

As another example, if we apply to one term in (12.1) the cubic transformation (10.22), then after a lot of work it is possible to obtain a general, rational series convergent for $p \in (0, 1)$. At $p = 1/2$ for instance, we get the series

$$\sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{353}{272}\right) \left(\frac{17}{2^{11}}\right)^n (44100n^3 - 30420n^2 - 1559n - 206) = \frac{8704}{\pi}.$$

However, it is important to note that not all transformations lead to series of type (12.46).

We give another general theorem for the $s = 1/2$ case here. If we apply a quadratic transformation to one argument of (12.1) and Euler’s transformation (6.32) to the other, the result is also a rational series with at most a quadratic surd on the right hand side. Once again convergence is easy to establish (the rate is $|z_0| = (1+k)(4k^2 - 3k + 1)/(4k)$), and the general solution recorded below is proven in exactly the same way as Theorem 12.5.

Theorem 12.6. For $k \in (\frac{\sqrt{41}-5}{8}, 1)$,

$$\begin{aligned} \sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{1-3k+2k^2-2k^3}{4k^2-3k+1}\right) \left(\frac{-(1+k)(4k^2-3k+1)}{64k}\right)^n (C_3n^3 + C_2n^2 + C_1n + C_0) \\ = \frac{8k^{3/2}(4k^2-3k+1)}{\pi}, \end{aligned} \tag{12.49}$$

where

$$\begin{aligned} C_3 &= \frac{4(k-1)^2}{k+1}(2k-1)(4k^2+3k+1)^2, \\ C_2 &= 12(k-1)(2k-1)(16k^4+k^2-1), \\ C_1 &= 288k^6 - 400k^5 + 102k^4 + 97k^3 - 93k^2 + 47k - 9, \\ C_0 &= 2(32k^6 - 44k^5 + 9k^4 + 16k^3 - 14k^2 + 6k - 1). \end{aligned}$$

Examples include

$$\sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{1}{3}\right) \left(\frac{-1}{36}\right)^n (1 - 3n - 84n^2 - 121n^3) = \frac{18\sqrt{3}}{\pi},$$

from $k = 1/3$, and when $k = 1/2$ (chosen so that C_3 vanishes),

$$\sum_{n=0}^{\infty} \binom{2n}{n}^2 P_n\left(\frac{1}{2}\right) \left(\frac{3}{128}\right)^n (3 + 14n) = \frac{8\sqrt{2}}{\pi}. \quad (12.50)$$

The formula (12.50) is particularly interesting, because although it fits the form of the $1/\pi$ series considered in Chapter 10 perfectly, it cannot be explained by the general theory there (its τ_0 is $iK(\sqrt{3}/2)/(2K(1/2))$, which is not a quadratic irrationality).

Just as in Chapter 10, we can produce ‘companion series’ using Legendre’s relation; one example is

$$\begin{aligned} \sum_{n=0}^{\infty} \binom{2n}{n}^2 \left(\frac{3}{128}\right)^n \left[14n(196n^2 + 196n - 3)P_{n-1}\left(\frac{1}{2}\right) \right. \\ \left. - (1372n^3 + 3024n^2 + 1631n + 375)P_n\left(\frac{1}{2}\right) \right] = \frac{400\sqrt{2}}{\pi}. \end{aligned}$$

Remark 12.5.1. One might wonder what happens if we set $a(z) = b(z)$ in (12.44). In the case of (12.47), as the quadratic transformation is effectively the degree 2 modular equation, any series thus produced would be subsumed under the theory in Chapter 10 with the choice $N = 2$, and where $\sqrt{\beta}$ could be taken as a singular value. See also Section 12.5.3.3 for more discussions. \diamond

12.5.2.2. *The $s = 1/4$ case.* Even though equation (12.1) holds for $s \in (0, 1)$, we see in the last two theorems that transformations need to be applied to the right hand side of (12.1) before Legendre’s relation can be used. Since many such transformations are modular in nature, we are again confined to $s \in \{1/2, 1/3, 1/4, 1/6\}$. We now consider the $s = 1/4$ case in (12.1). One strategy here is to transform the

right hand side of (12.1) in terms of K ; the transformation required is (7.29). The transformed expression is of type (12.44) and we solve for $a(z_0)^2 = 1 - b(z_0)^2$ in the notation there. Proceeding along the same lines as in the proof of Theorem 12.5, the following theorem can then be established:

Theorem 12.7. For $k \in (0, 1)$,

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n (\frac{3}{4})_n}{n!^2} P_n \left(\frac{(1+k)(1-4k+7k^2)}{(1-3k)(1+3k^2)} \right) \left(\frac{(1+k)(1-3k)(1+3k^2)}{(1+3k)^2} \right)^n \\ \times (C_3 n^3 + C_2 n^2 + C_1 n + C_0) = \frac{3\sqrt{2}(1+3k)^{5/2}(1+3k^2)}{(1+k)\pi}, \quad (12.51)$$

where

$$C_3 = \frac{16(k-1)^2 k^2}{(1+k)^2} (8 + 15k + 9k^2)^2, \\ C_2 = 48(k-1)k(8 - 15k + 27k^2 + 27k^3 + 81k^4), \\ C_1 = (4 - 33k + 45k^2)(4 - 17k + 17k^2 - 3k^3 + 63k^4), \\ C_0 = 3(1 - 3k)^4(1 + k + 2k^2).$$

An example of an identity produced by Theorem 12.7 is

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n (\frac{3}{4})_n}{n!^2} P_n \left(\frac{9}{7} \right) \left(\frac{21}{100} \right)^n (216 - 2385n - 108432n^2 + 80656n^3) = \frac{12600\sqrt{5}}{\pi}.$$

Note that we may also choose k for the right hand side of (12.51) to be rational.

Here is a trick: if the denominator of the argument in P_n is 0 at some k_0 , and at the same time the geometric term z_0 vanishes, then we may take the limit $k \mapsto k_0$ which gets rid of the Legendre polynomial altogether (note that the leading coefficient of P_n is $\binom{2n}{n} 2^{-n}$). In (12.51), this occurs when $k_0 = 1/3$. After taking the limit and eliminating the n^3 term using a hypergeometric differential equation (14.3), we recover the Ramanujan series (of the type (12.40))

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{4})_n (\frac{1}{2})_n (\frac{3}{4})_n}{n!^3} \left(\frac{32}{81} \right)^n (1 + 7n) = \frac{9}{2\pi}. \quad (12.52)$$

The same trick, applied to the series which follows from the cubic transformation mentioned in the $s = 1/2$ case, results in

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^3}{n!^3} \left(\frac{1}{4} \right)^n (1 + 6n) = \frac{4}{\pi}, \quad (12.53)$$

from the choice $p = (\sqrt{3} - 1)/2$; this formula originated from Ramanujan [164] and was first proven by Chowla.

12.5.2.3. *The $s = 1/3$ case.* This case is slightly trickier. An attempt to transform the right hand side of (12.1) in terms of K , as we did for the $s = 1/4$ case, results in exceedingly messy computations. Applying low degree modular equations to one of the ${}_2F_1$'s (as we did in the $s = 1/2$ case, for (12.47) essentially uses the degree 2 modular equation) does not give convergent series. Instead, we resort to a formula in [103],

$${}_2F_1\left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| x\right) = (1 + 8x)^{-1/4} {}_2F_1\left(\begin{matrix} \frac{1}{6}, \frac{5}{6} \\ 1 \end{matrix} \middle| \frac{1}{2} - \frac{1 - 20x - 8x^2}{2(1 + 8x)^{3/2}}\right),$$

to transform the right hand side of (12.1), then solve for $a(z_0)^2 = 1 - b(z_0)^2$ in the notation of (12.44), followed by applying the generalised Legendre relation (12.43) with $s = 1/3$. We succeed in obtaining the following theorem, where $\alpha(z_0) = k^3$, $\beta(z_0) = \left(\frac{1-k}{1+2k}\right)^3$.

Theorem 12.8. *For $k \in (0, 1)$,*

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} P_n \left(\frac{1 - 4k + 6k^2 - 4k^3 + 10k^4}{(1 - 2k - 2k^2)(1 - 2k + 4k^2)} \right) \left(\frac{(1 + k + k^2)(1 - 2k - 2k^2)(1 - 2k + 4k^2)}{(1 + 2k)^3} \right)^n \times (C_3 n^3 + C_2 n^2 + C_1 n + C_0) = \frac{\sqrt{3} (1 + 2k)^4 (1 - 2k + 4k^2)}{\pi}, \tag{12.54}$$

where

$$C_3 = \frac{9(k - 1)^2 k^2}{1 + k + k^2} (3 + 4k + 2k^2)^2 (3 + 2k + 4k^2)^2,$$

$$C_2 = 27(k - 1)k(9 - 18k + 10k^2 + 12k^3 + 60k^4 + 160k^5 + 240k^6 + 192k^7 + 64k^8),$$

$$C_1 = 9 - 144k + 540k^2 - 584k^3 + 314k^4 - 228k^5 - 1256k^6 - 1072k^7 + 768k^8 + 2560k^9 + 1280k^{10},$$

$$C_0 = 2(1 - 2k - 2k^2)^2 (1 - 10k + 12k^2 - 24k^3 + 16k^4 + 32k^6).$$

Note that in this case the right hand side contains a surd for rational k . When $k \rightarrow (\sqrt{3} - 1)/2$, we get the series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{1}{2})_n (\frac{2}{3})_n}{n!^3} \left(\frac{3(7\sqrt{3} - 12)}{2} \right)^n (5 - \sqrt{3} + 22n) = \frac{7 + 3\sqrt{3}}{\pi}.$$

12.5.2.4. *The $s = 1/6$ case.* It is also possible to produce a general series for this case, though the details required hours of computer algebra. The derivation is similar to the $s = 1/3$ case, and we use Goursat's result [103]

$${}_2F_1\left(\begin{matrix} \frac{1}{6}, \frac{5}{6} \\ 1 \end{matrix} \middle| \frac{1}{2} - \frac{1}{2} \sqrt{1 - \frac{64(1-t)t^3}{(9-8t)^3}}\right) = \left(1 - \frac{8t}{9}\right)^{\frac{1}{4}} {}_2F_1\left(\begin{matrix} \frac{1}{3}, \frac{2}{3} \\ 1 \end{matrix} \middle| t\right),$$

followed by the generalised Legendre relation for $s = 1/6$.

The general result is too lengthy to be included here. Just to find suitable x (in P_n) and z_0 , we need to solve for rational points on the curve $u^2 + v^2 = 10$. Having done so, the resulting series converges for $k \in (1/3, 1)$; the coefficient of n alone is a degree 24 polynomial in k . Even for $k = 1/2$, large integers are involved:

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{6})_n (\frac{5}{6})_n}{n!^2} P_n \left(\frac{2437}{2365} \right) \left(\frac{15136}{296595} \right)^n \left(710512440561n^3 - 118714528800n^2 - 19263658756n - 2627089880 \right) = \frac{1402894350\sqrt{39}}{\pi}.$$

With the limit $k \rightarrow (\sqrt{5} - 1)/2$, however, we recover the Ramanujan series

$$\sum_{n=0}^{\infty} \frac{(\frac{1}{6})_n (\frac{1}{2})_n (\frac{5}{6})_n}{n!^3} \left(\frac{4}{125} \right)^n (1 + 11n) = \frac{5\sqrt{15}}{6\pi}. \quad (12.55)$$

In the general series, the $1/\pi$ side is actually the square root of a quartic in k , and hence rational points on it may be found by the standard process [78] of converting it to a cubic elliptic curve (namely, $y^2 = 62208 + 3312x - 144x^2 + x^3$). It follows that there are infinitely many rational solutions. The smallest solution for k (in terms of the size of the denominator) which admits a rational right hand side is $k = 6029/8693$, and the resulting series involves integers of over 100 digits.

12.5.2.5. *Rarefied Legendre polynomials.* Factorisations of the type (12.44) for generating functions of rarefied Legendre polynomials are given in Chapter 11. Using partial differentiation techniques, we may also apply Legendre's relation to deduce parameter-dependent rational series for them. The algebra is formidable and we do not present the general forms here; only two examples are given to demonstrate their existence:

$$\begin{aligned} & \sum_{n=0}^{\infty} \frac{(\frac{1}{2})_n^2}{n!^2} P_{2n} \left(\frac{91}{37} \right) \left(\frac{5}{37} \right)^{2n} (3108999168n^3 - 3255264000n^2 - 75508700n + 24025) \\ &= \frac{896968800}{\pi}, \\ & \sum_{n=0}^{\infty} \frac{(\frac{1}{3})_n (\frac{2}{3})_n}{n!^2} P_{3n} \left(\frac{19}{3\sqrt{33}} \right) \frac{39887347500n^3 - 6141658302n^2 + 172862917n - 15262470}{(11\sqrt{33})^n} \\ &= \frac{442203651\sqrt{11}}{2\pi}. \end{aligned}$$

Under appropriate limits, the series involving P_{2n} again gives (12.52), while the one for P_{3n} recovers equation (12.55).

12.5.3. Orr-type theorems.

12.5.3.1. *A result from Bailey or Brafman.* There are other formulas, notably ones of Orr-type, which satisfy (12.44); an example was given by Bailey [26, equation (6.3) or (7.2)]:

$${}_4F_3\left(s, s, 1-s, 1-s \left| \frac{-x^2}{4(1-x)} \right. \right) = {}_2F_1\left(s, 1-s \left| x \right. \right) {}_2F_1\left(s, 1-s \left| \frac{x}{x-1} \right. \right). \quad (12.56)$$

Specialising Bailey's result using $s = 1/4$, we have

$$\frac{\pi^2}{4} {}_4F_3\left(\frac{1}{4}, \frac{1}{4}, \frac{3}{4}, \frac{3}{4} \left| \frac{-4x^4(1-x^2)^2}{(1-2x^2)^2} \right. \right) = K(x)K\left(\frac{x}{\sqrt{2x^2-1}}\right). \quad (12.57)$$

This formula also follows from setting $x = 0$, $s = 1/2$ in Brafman's formula (12.1). We try different transformations for the right hand side of (12.57), in order to find a suitable z_0 for which the two arguments are complementary, so the procedures leading up to (12.46) may be applied. Indeed, after using Euler's transformation (6.32) to both terms followed by a quadratic transformation, we obtain the equivalent formulation

$$\frac{\pi^2}{4} \sqrt{\frac{(1+z)(1+z')}{2z'}} {}_4F_3\left(\frac{1}{4}, \frac{1}{4}, \frac{3}{4}, \frac{3}{4} \left| \frac{z^4}{4(z^2-1)} \right. \right) = K\left(\sqrt{\frac{2z}{z+1}}\right)K\left(\sqrt{\frac{z'-1}{z'+1}}\right),$$

where at $z_0 = (-1)^{1/6}$ the arguments in the K 's are complementary (and correspond to argument $1/4$ in the ${}_4F_3$). Proceeding as we did for our previous results, Legendre's relation gives

$$\sum_{n=0}^{\infty} \binom{4n}{2n}^2 \binom{2n}{n} \frac{3 + 26n + 48n^2 - 96n^3}{2^{12n}} = \frac{2\sqrt{2}}{\pi}. \quad (12.58)$$

This time we do not have a more general rational series depending on a parameter, since there is only one free variable x in (12.56). For other values of z_0 , algebraic irrationalities are involved, for instance

$$\begin{aligned} & \sum_{n=0}^{\infty} \binom{4n}{2n}^2 \binom{2n}{n} (4(151 + 73\sqrt{5})n^3 - 96(3 + \sqrt{5})n^2 - (25 - \sqrt{5})n - 3) \\ & \times \left(\frac{17\sqrt{5} - 38}{2^6}\right)^n = \frac{38 + 17\sqrt{5}}{\pi}. \end{aligned}$$

We note that it is routine to obtain results contiguous to (12.57) (see Chapter 14). Two such contiguous relations give elegant variations of (12.58):

$$\begin{aligned} \sum_{n=0}^{\infty} \binom{4n}{2n}^2 \binom{2n}{n} \frac{1 - 48n^2}{(1 - 4n)^2 2^{12n}} &= \frac{2\sqrt{2}}{\pi}, \\ \sum_{n=0}^{\infty} \binom{4n}{2n}^2 \binom{2n}{n} \frac{3 + 32n + 48n^2}{(1 + 2n)^2 2^{12n}} &= \frac{8\sqrt{2}}{\pi}, \end{aligned} \tag{12.59}$$

where the second sum has been proven in [106, table 2] using creative telescoping.

In fact, using the same z_0 as in (12.58), we may invoke (12.56) instead of its specialisation (12.57), and appeal to the generalised Legendre relation. The result, and those contiguous to it, are rather neat and hold for $s \in (0, 1)$:

$$\begin{aligned} &\sum_{n=0}^{\infty} \frac{(s)_n^2 (1-s)_n^2}{\left(\frac{1}{2}\right)_n (1)_n^3} \frac{s(1-s) + 2(1-s+s^2)n + 3n^2 - 6n^3}{(1-2s)^2 4^n} \\ &= \sum_{n=0}^{\infty} \frac{(s)_n^2 (1-s)_n^2}{\left(\frac{3}{2}\right)_n (1)_n^3} \frac{s(1-s) + 2n + 3n^2}{4^n} \\ &= \sum_{n=0}^{\infty} \frac{(s)_n^2 (-s)_n^2}{\left(\frac{1}{2}\right)_n (1)_n^3} \frac{s^2 - 3n^2}{s 4^n} = \frac{\sin(\pi s)}{\pi}. \end{aligned} \tag{12.60}$$

These series generalise (12.58) and (12.59). For rational s , the rightmost term in (12.60) is algebraic; e.g. for $s = 1/6$ we get the rational series

$$\sum_{n=0}^{\infty} \binom{6n}{4n} \binom{6n}{3n} \binom{4n}{2n} \frac{25 - 108n^2}{(6n - 5)^2 2^{8n} 3^{6n}} = \frac{3}{5\pi}.$$

12.5.3.2. *Another result due to Bailey.* We can take [26, equation (6.1)] (or [179, (2.5.31)]), from which we find

$$\pi K\left(\frac{1}{\sqrt{2}}\right) {}_4F_3\left(\begin{matrix} \frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{3}{4} \\ \frac{1}{2}, \frac{1}{2}, 1 \end{matrix} \middle| 16x^2 x'^2 (x'^2 - x^2)^2\right) = (K(x) + K'(x)) K\left(\sqrt{\frac{1}{2} - xx'}\right). \tag{12.61}$$

To prepare this identity for Legendre’s relation so as to produce even just one rational series requires much work.

We apply the cubic modular equation (10.22) to the rightmost term in (12.61). Denoting the ${}_4F_3$ in (12.61) by G , we have

$$\begin{aligned} &\pi K\left(\frac{1}{\sqrt{2}}\right) (1 + 2p) G\left(\frac{16p^3(1+p)^3(2-p-p^2)(1+2p-4p^3-2p^4)^2}{(1+2p)^4}\right) \\ &= (K + K') \left(\sqrt{\frac{1}{2} - \frac{\sqrt{p^3(1+p)^3(2-p-p^2)}}{1+2p}}\right) K\left(\sqrt{\frac{p(2+p)^3}{(1+2p)^3}}\right). \end{aligned}$$

At $p = \frac{\sqrt{14}-\sqrt{2}-2}{4}$ (corresponding to $x^2 = (1 - k_7)/2$), the arguments in the two K 's coincide. We then compute the derivatives up to the 3rd order for the above equation. Note that as G satisfies a differential equation of order 4, higher order derivatives are not required; however, since the derivatives also contain the terms EK , E^2 and K^2 , we are not a priori guaranteed a solution. After a significant amount of algebra, we amazingly end up with the rational series

$$\sum_{n=0}^{\infty} \frac{\binom{4n}{2n} \left(\frac{1}{4}\right)_n^2}{(2n)!} \frac{5 + 92n + 3120n^2 - 4032n^3}{2^{8n}} = \frac{8}{K(1/\sqrt{2})} = \frac{32\sqrt{\pi}}{\Gamma(\frac{1}{4})^2}. \tag{12.62}$$

12.5.3.3. *Some related constants.* Using a different set of parameters ($\alpha = \beta = \gamma/2 = 1/4$ in [26, equation (6.3)]), we have

$$\frac{\pi^3}{(2xx')^{\frac{1}{2}} \Gamma^4(\frac{3}{4})} {}_3F_2\left(\begin{matrix} \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \\ \frac{1}{2}, \frac{3}{4} \end{matrix} \middle| \frac{(1 - 2x^2)^4}{16x^2(x^2 - 1)}\right) = (K(x) + K'(x))^2. \tag{12.63}$$

In this case, applying Legendre's relation straightaway does not give anything non-trivial, but if we apply a quadratic transform to the $K(x)$ term first, then for the two arguments in the K 's to be equal, we need to solve the equation $\sqrt{1 - x^2} = 2\sqrt{x}/(1 + x)$, which gives $x = \sqrt{2} - 1$. Subsequently we can use Legendre's relation to obtain

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{4}\right)_n^4}{(4n)!} (8(457 - 325\sqrt{2}))^n (7 + 20(11 + 6\sqrt{2})n) = \frac{28(82 + 58\sqrt{2})^{\frac{1}{4}} \pi^2}{\Gamma^4(\frac{1}{4})}.$$

More series of this type are possible at special values of t , which are in fact singular values; c.f. the equation solved above is precisely the one to solve for the 2nd singular value (because k_r and k'_r are related by the modular equation of degree r and satisfy $k_r^2 + k'^2_r = 1$). Therefore, to produce a series from (12.63) we do not need Legendre's relation; instead a single differentiation (in the same way Ramanujan series are produced in [46]) suffices. For example, using k_3 we obtain one series corresponding to $1/\pi$ and another to $1/K(k_3)^2$:

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{4}\right)_n^4}{(4n)!} (-144)^n (1 + 20n) = \frac{8\sqrt{2} \pi^2}{\Gamma(\frac{1}{4})^4}, \tag{12.64}$$

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{4}\right)_n^4}{(4n)!} (-144)^n (5 - 8n + 400n^2) = \frac{(\frac{2}{\sqrt{3}} - 1) 2^{\frac{49}{6}} \pi^5}{\Gamma(\frac{1}{3})^6 \Gamma(\frac{1}{4})^4}. \tag{12.65}$$

12.5.4. Concluding remarks. In equations (12.52), (12.53) and (12.55), we witness the ability of Legendre's relation to produce Ramanujan series which have linear (as opposed to cubic) polynomials in n . Series of the latter type are connected with singular values (more precisely, when $iK'(t)/K(t)$ is a quadratic irrationality), as is further supported by Remark 12.5.1 and Section 12.5.3.3. We take this connection slightly further here.

We can bypass the need for Brafman's formula completely and produce Ramanujan series of type (12.40) only using Legendre's relation and modular transforms. For instance, take the following version of Clausen's formula (10.19),

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| 4x^2(1-x^2)\right) = \frac{4}{\pi^2(1+x)}K(x)K\left(\frac{2\sqrt{x}}{1+x}\right), \quad (12.66)$$

where we have performed a quadratic transformation to get the right hand side. When $x^2 + 4x/(1+x)^2 = 1$, $x = \sqrt{2} - 1$, the 2nd singular value. At this x , we take a linear combination of the right hand side of (12.66) and its first derivative (since we know a Ramanujan series exists and involves no higher order derivatives), then apply Legendre's relation (12.42). The result is the series

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^3}{n!^3} (2(\sqrt{2}-1))^{3n} (1+(4+\sqrt{2})n) = \frac{3+2\sqrt{2}}{\pi},$$

which also follows from (12.48) under the limit $k \rightarrow \sqrt{2} - 1$. (Applying Legendre's relation to (12.66) and its derivatives when x is not a singular value results in the trivial identity $0 = 0$, perhaps as expected.)

Applying the quadratic transform twice (i.e. giving the modular equation of degree 4), followed by transforming the ${}_3F_2$ in (12.66) and using Legendre's relation, we recover Ramanujan's series

$$\sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\right)_n^3}{n!^3} \left(\frac{-1}{8}\right)^n (1+6n) = \frac{2\sqrt{2}}{\pi}. \quad (12.67)$$

For our final examples, using the degree 3 modular equation (10.22), we have

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| \frac{4p^3(1+p)^3(1-p)(2+p)}{(1+2p)^2}\right) = \frac{1}{1+2p}K\left(\frac{p^3(2+p)}{1+2p}\right)K\left(\frac{p(2+p)^3}{(1+2p)^3}\right).$$

From this and a similar identity with the ${}_3F_2$ transformed, we derive the Ramanujan series (12.53) as well as (12.55). This method seems to be a simple alternative to producing the Ramanujan series (12.40), since we only need to know the modular

equations and Legendre's relation; there is no need to find, say, singular values of the second kind as is required in the approach in Section 12.2.

12.5.4.1. *Computational notes.* While all the results presented here are rigorously proven, we outline a method to discover such results numerically on a computer algebra system. Take the right hand side function in (12.44) and compute a linear combination of its derivatives with coefficients A_i . Replace the elliptic integrals K, K', E, E' by X, X^2, X^4, X^8 respectively (the indices are powers of 2). Evaluate to several thousand decimal places at the appropriate z_0 and collect the coefficients in X . Solve for A_i so that Legendre's relation is satisfied (note all the terms such as KK', E^2 are separated as different powers of X). Finally, identify A_i with PSLQ.

Many of our (algebraically proven) identities required several hours of computer time due to the complexity of the calculations and the sheer number of steps which needed human direction. Computational shortcuts, in particular the chain rule, were applied partially manually in order to prevent overflows or out of memory errors. Our procedure may benefit (both symbolically and numerically) from automatic differentiation algorithms, but this has not been explored.

In the course of simplifying say $a'(z_0)$ in terms of a parameter k , the following numerical trick may be used to avoid excessive computer algebra. If we suspect a complicated expression actually simplifies down to a rational function in k , just prepare a generic rational function with enough coefficients (to be adjusted if the following procedure fails), then substitute in enough values of k and evaluate both the expression and the rational function to high precision. Solve for the coefficients and identify them using PSLQ, the Inverse Symbolic Calculator, or continued fractions.

Weighted Sum Formulas for Multiple Zeta Values

ABSTRACT. We present a unified approach which gives completely elementary proofs of weighted sum formulas for double zeta values. This approach also leads to new evaluations of sums involving the harmonic numbers, the alternating double zeta values, and the Mordell-Tornheim double sum. We discuss a heuristic for finding or dismissing the existence of similar simple sums. We also produce some new sums from recursions involving the Riemann zeta and the Dirichlet beta functions. Finally, we look at sum formulas of multiple zeta values of lengths greater than two, and use a simple experimental approach to simplify an impressive multiple zeta evaluation by Zagier.

13.1. Introduction

Multiple zeta values are a natural generalisation of the Riemann zeta function at the positive integers; we shall first only consider multiple zeta values of length 2 (or *double zeta values*), defined for integers $a \geq 2$ and $b \geq 1$ by

$$\zeta(a, b) = \sum_{n=1}^{\infty} \sum_{m=1}^{n-1} \frac{1}{n^a m^b}. \quad (13.1)$$

It is rather immediate from series manipulations that

$$\zeta(a, b) + \zeta(b, a) = \zeta(a)\zeta(b) - \zeta(a+b), \quad (13.2)$$

thus we can compute in closed form $\zeta(a, a)$, though it is not *a priori* obvious that many other multiple zeta values can be factored into Riemann zeta values. Euler was among the first to study multiple zeta values; indeed, he gave the sum formula (for $s \geq 3$)

$$\sum_{j=2}^{s-1} \zeta(j, s-j) = \zeta(s). \quad (13.3)$$

When $s = 3$, this formula reduces to the celebrated result $\zeta(2, 1) = \zeta(3)$, which has many other proofs [48]. Formula (13.3) itself may be shown in many ways, one of which uses partial fractions, telescoping sums and change of summation order,

which we present in Section 13.2. Given the ease with which formula (13.3) may be derived or even experimentally observed (see Section 13.4), it is perhaps surprising that a similar equation, with ‘weights’ 2^j inserted, was only first discovered in 2007 [154]:

$$\sum_{j=2}^{s-1} 2^j \zeta(j, s-j) = (s+1)\zeta(s). \quad (13.4)$$

Formula (13.4) was originally proven in [154] using the closed form expression for $\zeta(n, 1)$ (which follows from (13.2) and (13.3)), together with induction on shuffle relations – relations arising from iterated integration of generalised polylogarithms which encapsulate the multiple zeta values (see Chapter 9). Equation (13.4) has been generalised to more sophisticated weights other than 2^j using generating functions, and to lengths greater than 2 (see e. g. [109]).

In conjunction, (13.2), (13.3) and (13.4) can be used to find a closed form for $\zeta(a, b)$ for $a + b \leq 6$ (some of them have been found in Chapter 9). Indeed, it is a result Euler wrote down and first elucidated in [39] that all $\zeta(a, b)$ with $a + b$ odd may be expressed in terms of Riemann zeta value; by contrast, $\zeta(5, 3)$ is conjectured not reducible to more fundamental constants.

The third weighted sum we will consider is

$$\sum_{j=2}^{2s-1} (-1)^j \zeta(j, 2s-j) = \frac{1}{2} \zeta(2s). \quad (13.5)$$

Given that all known proofs of (13.4) had their genesis in more advanced areas, one purpose of this chapter is to show that (13.4) and the alternating (13.5) are not intrinsically harder than (13.3) and can be proven in a few short lines. We use the same techniques in Section 13.3 to give similar identities involving closely related functions. We also observe that some double zeta values sums are related to recursions (or convolutions) satisfied by the Riemann zeta function, a connection which we exploit in Section 13.4. We will use such recursions and a reflection formula to produce new results for character sums as defined in [58].

13.2. Elementary proofs

In the proofs below, the orders of summation may be interchanged freely, as the sums involved are absolutely convergent.

PROOF OF (13.4). We write the left hand side of (13.4) as

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

We consider the 2 cases, $m = n$ and $m \neq n$. In the former case the sum immediately yields $(s-2)\zeta(s)$. In the latter case, we do the geometric sum in j first to obtain

$$\sum_{\substack{m,n>0 \\ m \neq n}} \frac{2^s}{(n^2 - m^2)(n+m)^{s-2}} - \frac{4}{(n^2 - m^2)n^{s-2}}. \quad (13.6)$$

The first summand in (13.6) has antisymmetry in the variables m, n and hence vanishes when summed.

For the second term in (13.6), we use partial fractions to obtain

$$\sum_{\substack{m>0 \\ m \neq n}} \frac{1}{m^2 - n^2} = \frac{1}{2n} \sum_{\substack{m>0 \\ m \neq n}} \frac{1}{m-n} - \frac{1}{m+n} = \frac{3}{4n^2},$$

as the last sum telescopes (this is easy to see by first summing up to $m = 3n$, then looking at the remaining terms $2n$ at a time).

Therefore, summing over n in the second term of (13.6) gives $3\zeta(s)$. The result follows. \square

Our proof suggests that the base ‘2’ in the weighted sum is rather special as it induces antisymmetry. Another special case is obtained by replacing the 2 by a 1, and the same method proves Euler’s result.

PROOF OF (13.3). We apply the same procedure as in the previous proof and sum the geometric series first, so the left hand side becomes

$$\begin{aligned} & \sum_{m,n>0} \frac{1}{m(m+n)n^{s-2}} - \frac{1}{m(m+n)^{s-1}} = \sum_{n>0} \frac{1}{n^{s-1}} \sum_{m>0} \left(\frac{1}{m} - \frac{1}{m+n} \right) - \zeta(s-1, 1) \\ &= \sum_{n=1}^{\infty} \frac{1}{n^{s-1}} \sum_{k=1}^n \frac{1}{k} - \zeta(s-1, 1) = \sum_{n=1}^{\infty} \frac{1}{n^s} + \sum_{n=1}^{\infty} \frac{1}{n^{s-1}} \sum_{k=1}^{n-1} \frac{1}{k} - \zeta(s-1, 1) = \zeta(s), \end{aligned}$$

where we have used partial fractions for the first equality, and telescoping for the second. \square

Likewise we may easily prove the alternating sum (13.5):

PROOF OF (13.5). We write the left hand side out in full as above, then perform the geometric sum first to obtain

$$\sum_{m,n>0} \frac{1}{(m+n)(m+2n)n^{2s-2}} - \frac{1}{(m+2n)(m+n)^{2s-1}}.$$

Let $k = m + n$, so we have

$$\sum_{k>n>0} \frac{1}{k(k+n)n^{2s-2}} - \frac{1}{(k+n)k^{2s-1}}.$$

In the first term, use partial fractions and sum over k from $n+1$ to ∞ ; in the second term, sum over n from 1 to $k-1$. We get

$$\left(\sum_{n>0} \frac{1}{n^{2s-1}} \sum_{k=n+1}^{2n} \frac{1}{k} \right) - \left(\sum_{k>0} \frac{1}{k^{2s-1}} \sum_{n=k+1}^{2k-1} \frac{1}{n} \right).$$

It now remains to observe that if we rename the variables in the second bracket, then the two sums telescope to $\sum_{n>0} 1/(2n^{2s}) = \zeta(2s)/2$. Hence (13.5) holds. \square

Remark 13.2.1. The final sums we shall consider in this section are

$$\sum_{j=1}^{s-1} \zeta(2j, 2s-2j) = \frac{3}{4}\zeta(2s), \quad \sum_{j=1}^{s-1} \zeta(2j+1, 2s-2j-1) = \frac{1}{4}\zeta(2s). \quad (13.7)$$

These results were first given in [96] and later proven in a more direct manner in [152] using recursion of the Bernoulli numbers. The difference of the two equations in (13.7) is (13.5) and the sum is a case of (13.3). Therefore, the elementary nature of (13.7) is revealed since we have elementary proofs of (13.3) and (13.5).

If we add the first equation in (13.7) to itself but reverse the order of summation, then upon applying (13.2) we produce the identity

$$\sum_{j=1}^{s-1} \zeta(2j)\zeta(2s-2j) = \left(s + \frac{1}{2}\right)\zeta(2s), \quad (13.8)$$

which is usually derived from the generating function of the Bernoulli numbers B_n (13.44), since

$$2(2n)! \zeta(2n) = (-1)^{n+1} (2\pi)^{2n} B_{2n}. \quad (13.9)$$

\diamond

13.3. New sums

We shall see in this section that the elementary methods in Section 13.2 can in fact take us a long way.

13.3.1. Mordell-Tornheim Double Sum. The *Mordell-Tornheim double sum* (sometimes also known as the Mordell-Tornheim-Witten zeta function) is defined as

$$W(r, s, t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{n^r m^s (n+m)^t}.$$

Note that $W(r, s, 0) = \zeta(r)\zeta(s)$ and $W(r, 0, t) = W(0, r, t) = \zeta(t, r)$. Due to the simple recursion $W(r, s, t) = W(r-1, s, t+1) + W(r, s-1, t+1)$, when r, s, t are positive integers W may be expressed in terms of Riemann zeta or double zeta values (see e. g. [117]):

$$W(r, s, t) = \sum_{i=1}^r \binom{r+s-i-1}{s-1} \zeta(r+s+t-i, i) + \sum_{j=1}^s \binom{r+s-j-1}{r-1} \zeta(r+t+t-j, j).$$

We note also that by using a Laplace transform, $W(r, s, t)$ may be computed efficiently in terms of polylogs:

$$W(r, s, t) = \frac{1}{\Gamma(t)} \int_0^1 \text{Li}_r(x) \text{Li}_s(x) (-\log x)^{t-1} \frac{dx}{x}.$$

We again emulate the proof of (13.4) to obtain what seems to be a new sum over W .

Theorem 13.1. For integers $a \geq 0$ and $s \geq 3$,

$$\begin{aligned} \sum_{j=2}^{s-1} W(s-j, a, j) &= (-1)^a \zeta(s+a) + (-1)^a \zeta(s+a-1, 1) - \zeta(s-1, a+1) \\ &\quad - \sum_{i=2}^{a+1} (-1)^{i+a} \zeta(i) \zeta(s+a-i) \\ &= \sum_{i=2}^{s-1} \binom{i+a-2}{a} \zeta(i+a, s-i) + \sum_{i=s-a}^{s-1} \binom{i+a-2}{s-3} \zeta(i+a, s-i). \end{aligned} \tag{13.10}$$

PROOF. As the Mordell-Tornheim double sum values can be expressed as double zeta values, the second equality follows after simplification. For the first equality, we sketch the proof based on that of (13.4). Writing the left hand side of (13.10) as a triple sum, we perform the geometric sum first to produce

$$\sum_{m, n > 0} \frac{(-1)^a}{m^{a+1} n^{s-2} (m+n)} - \frac{(-1)^a}{m^{a+1} (m+n)^{s-1}}.$$

To the first term we apply the partial fraction decomposition

$$\frac{1}{m^b (m+n)} = \frac{(-1)^b}{n^b (m+n)} + \sum_{i=1}^b \frac{(-1)^{b-i}}{m^i n^{b+1-i}}.$$

We recognise the resulting sums as Riemann zeta and double zeta values. The result follows readily. \square

When $a = 0$ in (13.10), we recover (13.3); when $a = 1$, we obtain the pretty formula

Corollary 13.1.

$$\sum_{j=2}^s W(s-j, 1, j) = \zeta(2, s-1), \tag{13.11}$$

which, by the second equality in (13.10), is equivalent to

$$\sum_{j=2}^{s-1} j \zeta(j, s-j) = 2\zeta(s) + \zeta(2, s-1) - (s-2)\zeta(s-1, 1). \tag{13.12}$$

When $a = 2$ in (13.10), we have

$$\sum_{j=2}^s W(s-j, 2, j) = \zeta(s+2) + \zeta(s+1, 1) + \zeta(3, s-1) - \zeta(2, s).$$

A counterpart to (13.11) is the following alternating sum:

$$\sum_{j=2}^{2s} (-1)^j W(2s+1-j, 1, j) = \zeta(2s+1, 1) + \frac{1}{4}\zeta(2s+2), \tag{13.13}$$

and the same procedure can be used to prove this and to provide a closed form for the general case, i. e. the alternating sum of $W(s-j, a, j)$, though we omit the details but only provide one example:

$$\begin{aligned} & \sum_{j=2}^{2s} (-1)^j W(2s+1-j, 2a+1, j) \\ &= \sum_{j=1}^{2a} 2^{-j} \zeta(2s+j, 2a+2-j) + (-2)^{-j} (1-2^j) \zeta(2s+j) \zeta(2a+2-j) \\ & \quad + (1-3 \cdot 4^{-a-1}) \zeta(2a+2+2s) + \zeta(2a+1+2s, 1). \end{aligned}$$

Also, (13.12) is not an isolated result, for instance we have

$$\sum_{j=2}^{s-1} j^2 \zeta(j, s-j) = 3\zeta(s) + 3\zeta(2)\zeta(s-2) + 2\zeta(3, s-3) - s(s-2)\zeta(s-1, 1) - (2s-3)\zeta(s-2, 2).$$

Remark 13.3.1. There are other identities involving W that can be proven in an elementary manner. For instance, [117] records the sum

$$W(2n, 2n, 2n) = \frac{4}{3} \sum_{i=0}^n \binom{4n-2i-1}{2n-1} \zeta(2i) \zeta(6n-2i),$$

where $\zeta(0) = -1/2$; the existence of such a formula was first observed by Mordell. This sum can be proven by first expressing the left hand side as a sum of double zeta values, then by laboriously applying the partial fraction decomposition of $\zeta(s)\zeta(t)$ in terms of double zetas, as is used in [39]. \diamond

13.3.2. Sums Involving the Harmonic Numbers. The n th harmonic number is given by $H_n = \sum_{k=1}^n \frac{1}{k}$. If we replace $2s$ by $2s + 1$ in the proof of (13.5) (that is, when the sum of arguments in the double zeta value is odd instead of even), then we obtain

$$\frac{5}{2}\zeta(2s + 1) + 2\zeta(2s, 1) + \sum_{j=2}^{2s} (-1)^j \zeta(j, 2s + 1 - j) = 2 \sum_{n=1}^{\infty} \frac{H_{2n}}{n^{2s}}. \tag{13.14}$$

Combined with known double zeta values, we can evaluate the right hand side, giving

$$\sum_{n=1}^{\infty} \frac{H_{2n}}{n^4} = \frac{37}{4}\zeta(5) - \frac{2}{3}\pi^2\zeta(3),$$

etc, in agreement with results obtained via Mellin transform and generating functions in [58] (in whose notation such sums are related to $[2a, 1](2s, 1)$ – this notation is explained in Section 13.4). Indeed, replacing our right hand side with results in [58], we have:

$$\sum_{j=2}^{2s} (-1)^j \zeta(j, 2s + 1 - j) = (4^s - s - 2)\zeta(2s + 1) - 2 \sum_{k=1}^{s-1} (4^{s-k} - 1)\zeta(2k)\zeta(2s + 1 - 2k). \tag{13.15}$$

Similarly, using weight $\frac{1}{2}$ (instead of 2), we have another new result:

Lemma 13.1. *For integer $s \geq 3$,*

$$\begin{aligned} \sum_{j=2}^{s-1} 2^{1-j} \zeta(j, s - j) &= (2^{1-s} - 1)(\zeta(s - 1, 1) - 2 \log(2)\zeta(s - 1)) \\ &+ (2^{2-s} - 1)\zeta(s) + \sum_{n=0}^{\infty} \frac{H_n}{(2n + 1)^{s-1}}. \end{aligned} \tag{13.16}$$

Therefore, we may produce evaluations such as

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{H_n}{(2n + 1)^4} &= \frac{372\zeta(5) - 21\pi^2\zeta(3) - 2\pi^4 \log(2)}{96}, \\ \sum_{n=0}^{\infty} \frac{H_n}{(2n + 1)^5} &= \frac{\pi^6 - 294\zeta(3)^2 - 744 \log(2)\zeta(5)}{384}. \end{aligned}$$

Indeed, in (13.16) the harmonic number sum relates to the functions $[2a, 1]$ and $[2a, 2a]$ in [58], and when s is odd, we use their closed forms to simplify (13.16):

$$\sum_{j=2}^{2s} 2^{1-j} \zeta(j, 2s+1-j) = (s-1 + 2^{1-2s}) \zeta(2s+1) - \sum_{k=1}^{s-1} (4^{-k} - 4^{-s})(4^k - 2) \zeta(2k) \zeta(2s+1-2k). \quad (13.17)$$

On the other hand, if we chose even s in (13.16), then $[2a, 1]$, $[2a, 2a]$ seem not to simplify in terms of more basic constants, though below we manage to find a closed form for their difference (the proof here is more technical). Combined with (13.16), we have

Theorem 13.2. *For integer $s \geq 2$,*

$$\begin{aligned} \sum_{n=0}^{\infty} \frac{H_n}{(2n+1)^{2s-1}} &= (1-4^{-s})(2s-1)\zeta(2s) - (2-4^{1-s})\log(2)\zeta(2s-1) \\ &\quad + (1-2^{-s})^2\zeta(s)^2 - \sum_{k=2}^s 2(1-2^{-k})(1-2^{k-2s})\zeta(k)\zeta(2s-k); \end{aligned} \quad (13.18)$$

$$\begin{aligned} \sum_{j=2}^{2s-1} 2^{1-j} \zeta(j, 2s-j) &= \frac{1}{2}(1-2^{1-s})^2\zeta(s)^2 + \frac{1}{2}(2^{3-2s} + 2s-3)\zeta(2s) \\ &\quad - \sum_{k=2}^s (2^{k-1}-1)(2^{1-k}-4^{1-s})\zeta(k)\zeta(2s-k). \end{aligned} \quad (13.19)$$

PROOF. We only need to prove the first equality as the second follows from (13.16); to achieve this we borrow techniques from [58].

Using the fact that the harmonic number sum is $2([2a, 1](2s-1, t) - [2a, 2a](2s-1, t))$ in the notation of [58], we use the results therein (obtained using Mellin transforms) to write down its integral equivalent:

$$\sum_{n=0}^{\infty} \frac{H_n}{(2n+1)^{2s-1}} = \int_0^1 \frac{\log(x)^{2s-2} \log(1-x^2)}{\Gamma(2s-1)(x^2-1)} dx.$$

We denote its generating function by $F(w)$, and after interchanging orders of summation and integration, we obtain

$$\begin{aligned}
 F(w) &:= \sum_{s=2}^{\infty} \left[\int_0^1 \frac{\log(x)^{2s-2} \log(1-x^2)}{\Gamma(2s-1)(x^2-1)} dx \right] w^{2s-2} \\
 &= \int_0^1 \frac{x^{-w}(x^w-1)^2 \log(1-x^2)}{2(x^2-1)} dx \\
 &= -\frac{1}{2} \int_0^1 \frac{d}{dq} \left[x^{-w}(x^w-1)^2(1-x^2)^{q-1} \right]_{q=0} dx.
 \end{aligned}$$

Next, we interchange the order of differentiation and integration; the result is a Beta integral which evaluates to:

$$\begin{aligned}
 F(w) &= \frac{1}{4} \frac{d}{dq} \left[\frac{2\Gamma(1/2)\Gamma(q)}{\Gamma(q+1/2)} - \frac{\Gamma((1-w)/2)\Gamma(q)}{\Gamma((1-w)/2+q)} - \frac{\Gamma((1+w)/2)\Gamma(q)}{\Gamma((1+w)/2+q)} \right]_{q=0} \\
 &= \frac{1}{8} \left[8 \log(2)^2 - \pi^2 + \pi^2 \sec^2\left(\frac{\pi w}{2}\right) - \left[\Psi\left(\frac{1-w}{2}\right) + \gamma \right]^2 - \left[\Psi\left(\frac{1+w}{2}\right) + \gamma \right]^2 \right],
 \end{aligned}$$

where Ψ denotes the digamma function (5.24) and γ is the Euler-Mascheroni constant. The desired equality follows using the series expansions

$$\begin{aligned}
 -\Psi\left(\frac{1-w}{2}\right) &= \gamma + 2 \log(2) + \sum_{k=1}^{\infty} (2-2^{-k})\zeta(k+1)w^k, \\
 \frac{\pi^2}{2} \sec^2\left(\frac{\pi w}{2}\right) &= \sum_{k=0}^{\infty} (4-4^{-k})(2k+1)\zeta(2k+2)w^{2k}.
 \end{aligned}$$

□

Remark 13.3.2. Thus Theorem 13.2, together with [58], completes the evaluation of

$$\sum_{n=0}^{\infty} \frac{H_n}{(2n+1)^s}$$

in terms of well known constants for integer $s \geq 2$. In [13, theorem 6.5] it is claimed that said sum may be evaluated in terms of Riemann zeta values alone, but this is unsubstantiated by numerical checks, and notably $\log(2)$ is missing from the purported evaluation. ◇

Remark 13.3.3. Some evaluations relating to the digamma function appear in Chapter 5. More sums involving H_n can be found in the random walks chapters; indeed, the key result (3.66) was evaluated with the help of $[2a, 1](3, 1)$ and $[2a, 2a](3, 1)$ in [58]. ◇

13.3.3. Alternating Double Zeta Values. The *alternating* double zeta values $\zeta(a, \bar{b})$ are defined as

$$\zeta(a, \bar{b}) = \sum_{n=1}^{\infty} \sum_{m=1}^{n-1} \frac{1}{n^a} \frac{(-1)^{m-1}}{m^b},$$

with $\zeta(\bar{a}, b)$ and $\zeta(\bar{a}, \bar{b})$ defined similarly (the bar indicates the position of the -1). In [58], explicit evaluations of $\zeta(s, \bar{1}), \zeta(\bar{2s}, 1)$ and $\zeta(\bar{2s}, \bar{1})$ are given in terms of Riemann zeta values and $\log(2)$; in [39], it is shown that $\zeta(a, \bar{b})$ etc. with $a + b$ odd may be likewise reduced; small examples include (see also [48] for the first one)

$$\zeta(\bar{2}, 1) = -\frac{\zeta(3)}{8}, \quad \zeta(2, \bar{1}) = \frac{\pi^2 \log(2)}{4} - \zeta(3), \quad \zeta(\bar{2}, \bar{1}) = \frac{\pi^2 \log(2)}{4} - \frac{13\zeta(3)}{8}.$$

Again, if we follow closely the proof of (13.3), we arrive at new summation formulas such as

$$\sum_{j=2}^{s-1} \zeta(j, \overline{s-j}) = (1 - 2^{1-s})\zeta(s) + \zeta(\overline{s-1}, 1) + \zeta(\overline{s-1}, \bar{1}), \tag{13.20}$$

and so on. When s is odd, we simplify the right hand side using results in [58], thus:

$$\begin{aligned} \sum_{j=2}^{2s} \zeta(j, \overline{2s+1-j}) &= 2(1 - 4^{-s}) \log(2)\zeta(2s) - \zeta(2s+1) \\ &\quad + \sum_{k=1}^{s-1} (2^{1-2k} - 4^{k-s})\zeta(2k)\zeta(2s+1-2k), \\ \sum_{j=2}^{2s} (-1)^j \zeta(j, \overline{2s+1-j}) &= 2(1 - 4^{-s}) \log(2)\zeta(2s) + \left((s+1)4^{-s} - \frac{1}{2} - s \right) \zeta(2s+1) \\ &\quad + \sum_{k=1}^{s-1} (1 - 4^{k-s})\zeta(2k)\zeta(2s+1-2k). \end{aligned}$$

The last two formulas may be added or subtracted to give sums for even or odd j 's, for instance

$$\sum_{j=1}^{s-1} \zeta(2j+1, \overline{2s-2j}) = \left(\frac{2s-1}{4} - \frac{s+1}{2^{2s+1}} \right) \zeta(2s+1) - \sum_{k=1}^{s-1} \left(\frac{1}{2} - \frac{1}{4^k} \right) \zeta(2k)\zeta(2s+1-2k). \tag{13.21}$$

With perseverance, we may produce a host of similar identities for the three alternating double zeta functions. We only give some examples below; as they have similar proofs, we omit the details.

When we evaluate $\sum_{j=2}^{s-1} (\pm 1)^j \zeta(\bar{j}, s-j)$, we get for example

$$\begin{aligned} \sum_{j=2}^{s-1} \zeta(\bar{j}, s-j) &= (1 - 2^{1-s})(\zeta(s) + \zeta(s-1, 1) - 2 \log(2)\zeta(s-1)) \\ &\quad - \zeta(\overline{s-1}, 1) - \sum_{n=0}^{\infty} \frac{H_n}{(2n+1)^{s-1}}, \end{aligned}$$

and by applying (13.16) to the results, we obtain

$$\sum_{j=2}^{2s} (2^{1-j} \zeta(j, 2s+1-j) + \zeta(\bar{j}, 2s+1-j)) = 4^{-s} \zeta(2s+1) - \zeta(\overline{2s}, 1), \quad (13.22)$$

$$2 \sum_{j=1}^s \zeta(\overline{2j}, 2s+1-2j) = \frac{4^{-s} - 1}{2} \zeta(2s+1) - \zeta(\overline{2s}, 1), \quad (13.23)$$

where the right hand side of both equations may be reduced to Riemann zeta values by results in [58].

Likewise, for $\zeta(\bar{j}, \overline{s-j})$ we may deduce

$$\begin{aligned} \frac{1}{2} \sum_{j=2}^{2s} \zeta(\bar{j}, \overline{2s+1-j}) &= (1 - 4^{-s}) \log(2) \zeta(2s) - \frac{2s(2^{2s+1} - 1) - 1}{4^{s+1}} \zeta(2s+1) \\ &\quad + \sum_{k=1}^{s-1} (4^k - 1)(4^{-k} - 4^{-s}) \zeta(2k) \zeta(2s+1-2k); \quad (13.24) \end{aligned}$$

$$\begin{aligned} \sum_{j=1}^{s-1} \zeta(\overline{2j+1}, \overline{2s-2j}) &= \left(\frac{1}{2} (4^s - 3s - 2) + 4^{-s}(s+1) \right) \zeta(2s+1) \\ &\quad - \sum_{k=1}^{s-1} 4^{-(s+k)} (4^s - 4^k)^2 \zeta(2k) \zeta(2s+1-2k). \quad (13.25) \end{aligned}$$

Therefore, for the sums of the three alternating double zeta values, we have succeeded in giving closed forms when s (the sum of the arguments) is odd and the summation index j is odd, even, or unrestricted; it is interesting to compare this to the non-alternating case, whose sum is simpler when s is even (see Remark 13.2.1). A notable exception is the following formula, whose proof is similar to that of (13.5):

Theorem 13.3. *For integer $s \geq 2$,*

$$4 \sum_{j=1}^{s-1} \zeta(\overline{2j}, \overline{2s-2j}) = (4^{1-s} - 1) \zeta(2s). \quad (13.26)$$

Remark 13.3.4. Though it is believed that $\zeta(\bar{s}, 1)$ and $\zeta(\bar{s}, \bar{1})$ cannot be simplified in terms of well known constants for odd s , their difference can (this situation is analogous to Theorem 13.2 and can be proven using the same method):

$$\zeta(\bar{s}, 1) - \zeta(\bar{s}, \bar{1}) = (1 - 2^{-s})(s \zeta(s + 1) - 2 \log(2)\zeta(s)) - \sum_{k=1}^{s-2} (1 - 2^{-k})\zeta(k + 1)\zeta(s - k).$$

Moreover, some of the sums involving $\zeta(\bar{s}, 1)$ and $\zeta(\bar{s}, \bar{1})$ are much neater when the summation index j starts from 1 instead of 2, for instance

$$\begin{aligned} \sum_{j=1}^{s-1} \zeta(\bar{j}, s - j) &= (2^{2-s} - 1) \log(2)\zeta(s - 1) - \zeta(\overline{s-1}, 1), \\ \sum_{j=1}^{s-1} \zeta(\bar{j}, \overline{s-j}) &= \zeta(s - 1, \bar{1}) - \log(2)\zeta(s - 1), \\ 2 \sum_{j=1}^{2s} (-1)^j \zeta(\bar{j}, 2s + 1 - j) &= (2 - 4^{1-s}) \log(2)\zeta(2s) - (1 - 4^{-s})\zeta(2s + 1). \end{aligned}$$

◇

We wrap up this section with a surprising result, an alternating analog of (13.4):

Theorem 13.4. For integer $s \geq 3$,

$$\sum_{j=2}^{s-1} 2^j \zeta(\bar{j}, s - j) = (3 - 2^{2-s} - s)\zeta(s). \tag{13.27}$$

PROOF. The proof is very similar to that of (13.4): we write the left hand side as a triple sum and first take care of the $m = n$ case. Then we sum the geometric series to obtain

$$\sum_{\substack{m, n > 0 \\ m \neq n}} \frac{(-1)^{m+n} 2^s}{(m - n)(m + n)^{s-1}} - \frac{4(-1)^{m+n}}{(m - n)(m + n)n^{s-2}}.$$

The first term vanishes due to antisymmetry, and the second term telescopes:

$$\sum_{\substack{m > 0 \\ m \neq n}} \frac{(-1)^m}{m^2 - n^2} = \frac{2 + (-1)^n}{4n^2}.$$

Now summing over n proves the result. □

With (13.27) and results in [58], we can evaluate $\zeta(\bar{a}, b)$ etc. with $a + b = 4$, for instance

$$\zeta(\bar{2}, 2) = \frac{\log(2)^4}{6} - \frac{\log(2)^2 \pi^2}{6} + \frac{7 \log(2)\zeta(3)}{2} - \frac{13\pi^4}{288} + 4 \text{Li}_4\left(\frac{1}{2}\right). \tag{13.28}$$

13.4. More sums from recursions

In this section we first provide some experimental evidence which suggests that the sums in Section 13.2 (almost) exhaust all ‘simple’ and ‘nice’ sums in some sense. We then use a simple procedure which may be used to produce more weighted sums of greater complexity but of less elegance.

13.4.1. Experimental Methods. It is a curiosity why (13.4) had not been observed empirically earlier. As we can express all $\zeta(a, b)$ with $a + b \leq 7$ in terms of the Riemann zeta function, it is a simple matter of experimentation to try all combinations of the form

$$\sum_j (a \cdot b^j + c^s \cdot d^j) \zeta(j, s - j) = f(s) \zeta(s), \quad (13.29)$$

with j or s being even, odd or any integer (so there are 9 possibilities), $a, b, c, d \in \mathbb{Q}$, and $f : \mathbb{N} \rightarrow \mathbb{Q}$ is a (reasonable) function to be found.

Now if we assume that $\pi, \zeta(3), \zeta(5), \zeta(7), \dots$ are algebraically independent over \mathbb{Q} (which is widely believed to be true, though proof-wise we are a long way off, for instance, apart from π only $\zeta(3)$ is known to be irrational – see [187], and also Remarks 2.3.4 and 6.3.3), then we can substitute a few small values of s into (13.29) and solve for a, b, c, d in that order.

For instance, assuming a formula of the form $\sum_{j=2}^{s-1} a^j \zeta(j, s - j) = f(s) \zeta(s)$ holds, using $s = 5$ forces us to conclude that $a = 1$ or $a = 2$.

Indeed, when we carry out the experiment outlined above, it is revealed that the sums (13.3), (13.4), (13.5) are essentially the only ones in the form of (13.29), except for the case

$$\sum_{j=1}^{s-1} (d^j + d^{s-j}) \zeta(2j, 2s - 2j),$$

(note the factor in front of the ζ has to be invariant under $j \mapsto s - j$). Here, the choice of $d = 4$ leads to

$$\sum_{j=1}^{s-1} (4^j + 4^{s-j}) \zeta(2j, 2s - 2j) = \left(s + \frac{4}{3} + \frac{2}{3} 4^{s-1} \right) \zeta(2s),$$

a result which first appeared in [152] and was proven using the generating function of Bernoulli polynomials (see Section 13.5).

Remark 13.4.1. As noted in [152], more general constructions stemming from Bernoulli polynomials lead to non-closed form on the right hand sides, for instance

$$\sum_{j=1}^{s-1} (9^j + 9^{s-j}) \zeta(2j, 2s - 2j) = \frac{3(9^s + 3) + 8s}{8} \zeta(2s) + \frac{(6s - 5)(-1)^s (2\pi)^{2s}}{24(2s - 1)!} + \sum_{j=1}^{s-1} \frac{(-4\pi^2)^{s-j} 9^j}{6(2s - 2j - 1)!} \zeta(2j).$$

◇

Sums of the form

$$\sum_j p(s, j) \zeta(j, s - j) = f(s) \zeta(s),$$

where p is a non-constant 2-variable polynomial with rational coefficients, can also be subject to experimentation. If the degree of p is restricted to 2, then $j(s - j) \zeta(2j, 2s - 2j)$ is the only candidate which can give a closed form. Indeed, this sum was essentially considered in [152], using the identity

$$6 \sum_{j=2}^{s-2} (2j - 1)(2s - 2j - 1) \zeta(2j) \zeta(2s - 2j) = (s - 3)(4s^2 - 1) \zeta(2s). \tag{13.30}$$

The identity was due to Ramanujan [15, chapter 15, formula (14.2)]. Applying (13.2), the result can be neatly written as

$$\sum_{j=2}^{s-2} (2j - 1)(2s - 2j - 1) \zeta(2j, 2s - 2j) = \frac{3}{4} (s - 3) \zeta(2s). \tag{13.31}$$

Ramanujan’s identity above, and below – (13.32) – are actually more general than what is shown here, for they are identities between Eisenstein series of different weights. However, the forms shown here are routine to prove, as we outline in Section 13.5.

Searches for ‘simple’ weighted sums of length 3 multiple zeta values, and for q -analogs of (13.4), have so far proved unsuccessful (except for [67] which contains a generalisation of (13.5), see (13.50)).

13.4.2. Recursions of the Zeta Function. We observe that any recursion of the Riemann zeta values – or of Bernoulli numbers via (13.9) – of the form

$$\sum_j g(s, j) \zeta(2j) \zeta(2s - 2j)$$

for some function g would lead to a sum formula for double zeta values, due to (13.2). This was the idea behind (13.31) and was also hinted at in Remark 13.2.1, (13.8). We flesh out the details in some examples below.

One such recursion is [15, chapter 15, formula (14.14)], which can be written as

$$\begin{aligned} & \sum_{j=1}^{n-1} j(2j+1)(n-j)(2n-2j+1)\zeta(2j+2)\zeta(2n-2j+2) \\ &= \frac{1}{60}(n+1)(2n+3)(2n+5)(2n^2-5n+12)\zeta(2n+4) - \frac{\pi^4}{15}(2n-1)\zeta(2n). \end{aligned} \quad (13.32)$$

Upon applying (13.2) to the recursion, we obtain the new sum:

Theorem 13.5. *For integer $n \geq 4$,*

$$\begin{aligned} & \sum_{j=2}^{n-2} (j-1)(2j-1)(n-j-1)(2n-2j-1)\zeta(2j, 2n-2j) \\ &= \frac{3}{8}(n-1)(3n-2)\zeta(2n) - 3(2n-5)\zeta(4)\zeta(2n-4). \end{aligned} \quad (13.33)$$

Next, we use a result from [149], which states

$$\sum_{k=1}^{n-1} \left[1 - \binom{2n}{2k} \right] \frac{B_{2k} B_{2n-2k}}{(2k)(2n-2k)} = \frac{H_{2n}}{n} B_{2n}. \quad (13.34)$$

We apply (13.2) to the left hand side to obtain a sum of double zeta values; unfortunately one term of the sum involves $\sum_{k=1}^{n-1} (2k-1)!(2n-2k-1)!$ which has no nice closed form. On the other hand, a twin result in [144] gives

$$\sum_{k=1}^{n-2} \left[n - \binom{2n}{2k} \right] B_{2k} B_{2n-2k-2} = (n-1)(2n-1)B_{2n-2}. \quad (13.35)$$

When we apply (13.2) to it, we end up with a sum involving $\sum_{k=1}^{n-2} (2k)!(2n-2k-2)!$, which again has no nice closed form.

Yet, it is straight-forward to show by induction that

$$\sum_{k=0}^m \frac{(-1)^k}{\binom{n}{k}} = \frac{(n+1)! + (-1)^m(m+1)!(n-m)!}{(n+2)n!},$$

hence, when $m = n$, the sum vanishes if n is odd and equates to $2(n+1)/(n+2)$ when n is even. In other words, $\sum_{k=0}^{2n} (-1)^k k!(2n-k)!$ has a closed form, and accordingly we subtract the sums obtained from (13.34) and (13.35) to produce:

Proposition 13.1. *For integer $n \geq 2$,*

$$\begin{aligned} & \sum_{k=1}^{n-1} \left\{ \left[1 - \frac{1}{\binom{2n+2}{2k}} \right] \frac{n+1}{k(n+1-k)} \zeta(2k, 2n+2-2k) + \frac{\zeta(2n+2)}{\zeta(2n)} \times \right. \\ & \left. \left[\frac{2}{(2n+1)\binom{2n}{2k}} - \frac{(2k-n)^2 + (n+1)(n+2)}{(n-k+1)(2n-2k+1)(k+1)(2k+1)} \right] \zeta(2k, 2n-2k) \right\} \\ & = 3 \left[H_{2n-1} - H_{n-1} - \frac{2n^2+n+1}{2n(2n+1)} \right] \zeta(2n+2) - \frac{2n+3}{2n+1} \zeta(2n, 2). \end{aligned} \tag{13.36}$$

Our next result uses [4, equation (7.2)], whose special case gives:

$$B_n^2 + \frac{B_{2n}}{\binom{2n}{n}} = \frac{4n n!}{(2\pi)^{2n}} \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(2n-2k)!}{(n-k)(n-2k)!} \zeta(2k) \zeta(2n-2k). \tag{13.37}$$

Upon applying (13.2) and much algebra, we arrive at:

Proposition 13.2. *For integer $n \geq 2$,*

$$\begin{aligned} & \sum_{k=1}^{n-1} \frac{(n+|n-2k|)!}{(n+|n-2k|)|n-2k|!} \zeta(2k, 2n-2k) \\ & = \left[\frac{(1+(-2)^{1-n})(n-1)!}{4} + \frac{3(2n-1)!}{2n!} - \frac{(2n+1)!}{n(n+1)!} {}_2F_1 \left(\begin{matrix} 1, 2n+2 \\ n+2 \end{matrix} \middle| -1 \right) \right] \zeta(2n). \end{aligned}$$

PROOF. The only non-trivial step to check here is that the claimed ${}_2F_1$ is produced when we sum the fraction in (13.37); that is, we wish to prove the claim

$$\sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^n n \binom{2n-2k}{n-2k}}{2(n-k)} = \frac{1}{(1-x)^{n+1}} - x^m \binom{n+m}{n} {}_2F_1 \left(\begin{matrix} 1, n+m+1 \\ m+1 \end{matrix} \middle| x \right) \Big|_{x=-1, m=n+1}.$$

Our proof is quite experimental in nature. We observe that for x near the origin the right hand side is simply $\sum_{k=0}^{m-1} x^k \binom{n+k}{k}$, as they have the same recursion and initial values in m , hence when $x = -1$ they also agree by analytic continuation. This sum (in the limit $x = -1, m = n + 1$), as a function of n , also satisfies the recursion

$$4f(n) - 2f(n-1) = 3(-1)^n \binom{2n}{n}, \quad f(1) = -1,$$

which is the same recursion for the sum on the left hand side of the claim – as may be checked using Celine’s method [161]. Thus equality is established. \square

Remark 13.4.2. It is clear that a large number of (uninteresting) identities similar to the those recorded in the two propositions may be easily produced. Using [4,

(7.2) with $k = n + 1$], for instance, a very similar proof to the above gives

$$\sum_{k=1}^{n-1} \frac{4(n+1+|n-2k|)!}{n!(1+|n-2k|)!} \zeta(2k, 2n-2k) = (1+(-1)^n)(1-n)\zeta(n)^2 + \zeta(2n) \times \left\{ n+3 + (-1)^n(n-1+2^{-n}) + 2 \binom{2n+1}{n} \left[3 - \frac{4(2n+3)}{n+1} {}_2F_1 \left(\begin{matrix} 1, 2n+4 \\ n+3 \end{matrix} \middle| -1 \right) \right] \right\}.$$

Care must be exercised when consulting the literature, however, as we found in the course of this work that many recorded recursions of the Bernoulli numbers (or of the even Riemann zeta values) are in fact combinations and reformulations of the formula behind (13.31) and the basic identity appearing in Remark 13.2.1. \diamond

13.4.3. The Reflection Formula. Formula (13.2) is but a special case of a more general *reflection formula*. To state the reflection formula, we will need some notation from [58], which we have tried to avoid until now to keep the exposition elementary.

Let $\chi_p(n)$ denote a 4-periodic function on n ; for different p 's we tabulate values of χ_p below:

$p \setminus n$	1	2	3	4
1	1	1	1	1
$2a$	1	0	1	0
$2b$	1	-1	1	-1
-4	1	0	-1	0

We now define the series L_p by

$$L_p(s) = \sum_{n=1}^{\infty} \frac{\chi_p(n)}{n^s},$$

and $L_{pq}(s)$ means $\sum_{n>0} \chi_p(n)\chi_q(n)/n^s$. Finally, we define *character sums*, which generalise the double zeta values, by

$$[p, q](s, t) = \sum_{n=1}^{\infty} \sum_{m=1}^{n-1} \frac{\chi_p(n)}{n^s} \frac{\chi_q(m)}{m^t}. \tag{13.38}$$

In this notation, $\zeta(s, t) = [1, 1](s, t)$, $\zeta(s, \bar{t}) = [1, 2b](s, t)$, etc. We can now state the reflection formula [58, equation (1.7)]:

$$[p, q](s, t) + [q, p](t, s) = L_p(s)L_q(t) - L_{pq}(s+t). \tag{13.39}$$

Remark 13.4.3. With the exception of χ_{2b} , χ_p are examples of Dirichlet characters and L_p are the corresponding Dirichlet L -series. Indeed,

$$L_1(s) = \zeta(s), \quad L_{2a}(s) = (1 - 2^{-s})\zeta(s) = \lambda(s),$$

$$L_{2b}(s) = (1 - 2^{1-s})\zeta(s) = \eta(s), \quad L_{-4}(s) = \beta(s),$$

where the last three are the Dirichlet lambda, eta and beta functions respectively. We have implicitly used these series in the evaluation of lattice sums at the end of Chapter 7.

Moreover, $2(2n)! \beta(2n + 1) = (-1)^n (\pi/2)^{2n+1} E_{2n}$ for non-negative integer n , where E_n denotes the n th Euler number. Using generating functions, one may deduce convolution formulas for the Euler numbers, an example of which is

$$\sum_{k=0}^{n-2} \binom{n-2}{k} E_k E_{n-2-k} = 2^n (2^n - 1) \frac{B_n}{n}.$$

Many of our results in the previous sections would look neater had we used $\lambda(s)$ and $\eta(s)$ instead of $\zeta(s)$. ◇

Remark 13.4.4. In [89], it is shown that for $s + t$ even, the sum $[-4, 1](s, t) - [-4, 2b](s, t)$ may be evaluated in closed form. (In the notation of [89], this sum is $2^{t-1} G_{t,s}^{+-}$.)

The other sum considered in [89] is not found in [58], though we may apply the techniques used in the latter for small s, t , e. g. we have

$$G_{1,1}^{--} := \sum_{k=0}^{\infty} \sum_{j=1}^k \frac{(-1)^{j+k+1}}{(2k+1)j} = \frac{\pi}{4} \log(2) - G,$$

where $G = \beta(2)$ again denotes Catalan’s constant (see Chapter 5). General result are proven in [89] using integral transforms of Bernoulli identities. ◇

Using the standard convolution formulas of the Bernoulli and the Euler polynomials, and aided by the reflection formula (13.39), we can produce the following sums for $[p, q](s, t)$ as we did for $\zeta(s, t)$.

Theorem 13.6. *Using the notation of (13.38), we have, for integer $n \geq 2$,*

$$2 \sum_{k=1}^{n-1} [1, 2b](2k, 2n - 2k) + [2b, 1](2k, 2n - 2k) = -4 \sum_{k=1}^{n-1} [2b, 2b](2k, 2n - 2k)$$

$$= (1 - 4^{1-n})\zeta(2n); \tag{13.40}$$

$$\begin{aligned}
& 4 \sum_{k=1}^{n-1} [2a, 2a](2k, 2n-2k) = -4 \sum_{k=0}^{n-1} [-4, -4](2k+1, 2n-1-2k) \\
& = \sum_{k=1}^{n-1} [1, 2a](2k, 2n-2k) + [2a, 1](2k, 2n-2k) = (1-4^{-n})\zeta(2n); \quad (13.41)
\end{aligned}$$

$$\begin{aligned}
& \sum_{k=1}^n [2a, -4](2k, 2n+1-2k) + [-4, 2a](2n+1-2k, 2k) \\
& = \sum_{k=1}^{n-1} [2a, 2b](2k, 2n-2k) + [2b, 2a](2n-2k, 2k) = 0; \quad (13.42)
\end{aligned}$$

$$\begin{aligned}
& 2 \sum_{k=1}^n [1, -4](2k, 2n+1-2k) + [-4, 1](2n+1-2k, 2k) \\
& = -2 \sum_{k=1}^n [2b, -4](2k, 2n+1-2k) + [-4, 2b](2n+1-2k, 2k) \\
& = \beta(2n+1) + (16^{-n} - 2^{-1-2n})\pi \zeta(2n), \quad (13.43)
\end{aligned}$$

We note that (13.40) concerns the alternating double zeta values studied in Section 13.3 (c.f. the more elementary Theorem 13.3). As mentioned before, the identities above rest on well-known recursions, for instance the second equality in (13.42) is equivalent to the recursion

$$\sum_{k=1}^n \beta(2n+1-2k)\lambda(2k) = n\beta(2n+1).$$

Also, the many pairs of equalities within each numbered equation in the theorem are not all coincidental but stem from the identity in [58]:

$$[1, q] + [2b, q] = 2[2a, q],$$

where $q = 1, 2a, 2b$ or -4 .

Moreover, one can show the following equations; as character sums are not the main object of our study, we omit the details:

$$\begin{aligned}
& \sum_{k=1}^n 4^{-k} ([-4, 1](2n+1-2k, 2k) + [1, -4](2k, 2n+1-2k)) \\
&= \frac{1+2^{1-2n}}{6} \beta(2n+1) + (2^{-1-4n} - 4^{-1-n}) \pi \zeta(2n), \\
& \sum_{k=1}^{n-1} 4^k ([2a, 1](2k, 2n-2k) + [1, 2a](2n-2k, 2k)) \\
&= \frac{(1-4^{-n})(8+4^n)}{6} \zeta(2n).
\end{aligned}$$

Since there is an abundance of recursions involving the Bernoulli and the Euler numbers (see e.g. [157]), many more such identities may be produced using the reflection formula.

13.5. Length 3 and higher multiple zeta values

Earlier in this chapter, we made use of the properties of the Bernoulli numbers B_n , defined by the generating function

$$F(t) := \sum_{n=0}^{\infty} B_n \frac{t^n}{n!} = \frac{t}{e^t - 1}. \quad (13.44)$$

Note that $B_n = 0$ when n is odd (unless $n = 1$). The Bernoulli numbers are generalised to the Bernoulli polynomials $B_n(x)$, defined by the generating function

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

from which we see $B_n = B_n(0)$ (or $B_n(1)$, if we ignore B_1). The generating functions also give $B_n(1/2) = (2^{1-n} - 1)B_n$ when n is even, a property we have implicitly used.

Two of Ramanujan's identities used earlier involve the sums of $j(n-j) \binom{2n}{2j} B_{2j} B_{2n-2j}$ and $(j-1)(2j-1)(n-j-1)(2n-2j-1) \binom{2n}{2j} B_{2j} B_{2n-2j}$, respectively. We demonstrate that once such an identity is found, it can be proven routinely. The example below does just that to prove the first identity.

Example 13.5.1 (Proof of equation (13.30)). Via the connection

$$2(2n)! \zeta(2n) = (-1)^{n+1} (2\pi)^{2n} B_{2n}$$

(itself provable using, say, contour integration), we write (13.30) in the form

$$\sum_{j=1}^{n-1} j(n-j) \binom{2n}{2j} B_{2j} B_{2n-2j} = \frac{1}{24} (2n(2n-1)(2n-3)B_{2n-2} - (2n+1)(2n)(2n-1)B_{2n}).$$

We note that the left hand side is simply the coefficients of the square of the exponential generating function for jB_{2j} . Thus its generating function is easily obtained by differentiating $t/(e^t - 1)$ (after subtracting the term corresponding to B_1). The factorised right hand side lends itself easily as the coefficients of a combination of repeated derivatives of $t/(e^t - 1)$.

To be more precise, recall the notation $F(t) = t/(e^t - 1)$. Then the exponential generating function for the left hand side is

$$G_1(t) = \frac{t^2}{4} \left(F'(t) + \frac{1}{2} \right)^2,$$

while the generating function for the right hand is slightly more involved, for we first subtract off lower order terms since (13.30) does not hold when $n < 2$; it turns out to be

$$G_2(t) = \frac{t^4}{288} + \frac{t^4}{24} \frac{d}{dt} \left(\frac{F(t) - h(t)}{t} \right) - \frac{t^2}{24} \frac{d^3}{dt^3} (t(F(t) - h(t))),$$

where $h(t) = 1 - t/2 + t^2/12$. It remains to check that $G_1(t) \equiv G_2(t)$. ◇

Ramanujan’s second identity (13.32) is proven almost as routinely, except that for the corresponding right hand side, the irreducible factor $2n^2 - 13n + 30$ appears. To facilitate computation, this factor could be broken up as $n(n-2) + (n-5)(n-6)$, with each piece being viewed as an appropriate derivative.

Example 13.5.2 (A length 3 sum). By taking the cube of the generating function $t/(e^t - 1)$, we observe the routinely verified identity

$$\sum_{\substack{a,b,c>0 \\ a+b+c=n}} \binom{2n}{2a, 2b, 2c} B_{2a} B_{2b} B_{2c} = (n+1)(2n+1)B_{2n} + n \left(n - \frac{1}{2} \right) B_{2n-2}. \quad (13.45)$$

When translated into zeta terms, this is

$$4 \sum_{\substack{a,b,c>0 \\ a+b+c=n}} \zeta(2a)\zeta(2b)\zeta(2c) = (n+1)(2n+1)\zeta(2n) - \pi^2 \zeta(2n-2). \quad (13.46)$$

By either elementary sum manipulations, or by the harmonic relations (a.k.a. the stuffle product [114, 115]), we have

$$\zeta(r)\zeta(s)\zeta(t) = \left(\sum_{\text{sym}} \zeta(r, s, t)\right) + [\zeta(r)\zeta(s+t) + \zeta(s)\zeta(r+t) + \zeta(t)\zeta(r+s)] - 2\zeta(r+s+t), \tag{13.47}$$

where the first term on the right is a symmetric sum in r, s and t . The multiple zeta value $\zeta(r, s, t)$ has been defined in (9.2).

We sum both side of (13.47) over even r, s, t . After some simple combinatorics, the right hand side becomes

$$6 \sum_{a+b+c=n} \zeta(2a, 2b, 2c) + \frac{3}{4}(2n+1)(n-2)\zeta(2n) - (n-1)(n-2)\zeta(2n).$$

Consequently, by (13.46) we have

$$\sum_{a+b+c=n} \zeta(2a, 2b, 2c) = \frac{5}{8}\zeta(2n) - \frac{1}{4}\zeta(2)\zeta(2n-2). \tag{13.48}$$

This result first appeared in [67], though our derivation here is slightly more elementary. We now look at the alternating sum, also first studied in [67]:

$$\sum_{\substack{a+b+c=2n \\ a-1, b, c > 0}} ((-1)^a + (-1)^b + (-1)^c)\zeta(a, b, c).$$

When any of a, b, c is odd, the factor in front of the multiple zeta value returns -1 ; otherwise it returns 3. Thus, we can add this sum to Granville’s theorem [105]

$$\sum_{\substack{a_1+a_2+\dots+a_k=n \\ a_1-1, a_2, \dots, a_k > 0}} \zeta(a_1, a_2, \dots, a_k) = \zeta(n), \tag{13.49}$$

and apply (13.48), to find

$$\sum_{\substack{a+b+c=2n \\ a-1, b, c > 0}} ((-1)^a + (-1)^b + (-1)^c)\zeta(a, b, c) = \frac{3}{2}\zeta(2n) - \zeta(2)\zeta(2n-2). \tag{13.50}$$

◇

The authors of [67] also use a closed form formula for

$$\sum_{a+b+c+d=n} \binom{2n}{2a, 2b, 2c, 2d} B_{2a}B_{2b}B_{2c}B_{2d},$$

together with Ramanujan’s formula (13.30) to give the length 4 identity

$$\sum_{a+b+c+d=n} \zeta(2a, 2b, 2c, 2d) = \frac{35}{64}\zeta(2n) - \frac{5}{16}\zeta(2)\zeta(2n-2). \tag{13.51}$$

While [67] comments that the length 4 analogue of (13.50) would be difficult to find (our experiments indicate that it does not seem to have a closed form in terms of a rational multiple of π^{2n}), we can find other analogs, by performing a trick similar to that used in the derivation of (13.50). That is, we find a factor (a symmetric function of a, b, c, d) which returns -1 when either 2 or 4 of a, b, c, d are odd; we then combine it with (13.49). There are many choices here, one possibility being

Proposition 13.3. *For integer $n \geq 3$,*

$$\begin{aligned} & \sum_{\substack{a+b+c+d=2n \\ a-1, b, c, d > 0}} \left[2((-1)^a + (-1)^b + (-1)^c + (-1)^d) - (-1)^{abcd} \right] \zeta(a, b, c, d) \\ &= \frac{3}{16} \zeta(2n) - \frac{5}{4} \zeta(2) \zeta(2n-2). \end{aligned} \tag{13.52}$$

Clearly more results like the above are possible. We move onto a sum of a different form. Using formula (5) in [88] (which can again be easily proven, though slightly harder to discover – see Lemma 13.2),

$$\begin{aligned} & \sum_{\substack{a+b+c=n \\ a, b, c > 1}} (2a-1)(2b-1)(2c-1) \zeta(2a) \zeta(2b) \zeta(2c) \\ &= \frac{2n-5}{120} (6\pi^4 \zeta(2n-4) + (n-6)(n+1)(2n-1)(2n+1) \zeta(2n)), \end{aligned} \tag{13.53}$$

we ultimately deduce a three dimensional analogue of Nakamura’s identity (13.31),

Proposition 13.4. *For integer $n \geq 3$,*

$$\begin{aligned} & \sum_{\substack{a+b+c=n \\ a, b, c > 0}} (2a-1)(2b-1)(2c-1) \zeta(2a, 2b, 2c) \\ &= (2n-5) \zeta(4) \zeta(2n-4) - \frac{3(2n-3)}{4} \zeta(2) \zeta(2n-2) + \frac{8n-5}{8} \zeta(2n). \end{aligned} \tag{13.54}$$

PROOF. The proof proceeds along similar lines as our prior results. We first use (13.47), replace r by $2a$, s by $2b$, and t by $2c$, where $a + b + c = n$, then multiply both sides by $(2a-1)(2b-1)(2c-1)$, and sum over all positive integers a, b and c .

This gives

$$\begin{aligned}
 & 6 \sum_{\substack{a+b+c=n \\ a,b,c>0}} (2a-1)(2b-1)(2c-1)\zeta(2a, 2b, 2c) \\
 = & \sum_{\substack{a+b+c=n \\ a,b,c>0}} \left\{ (2a-1)(2b-1)(2c-1)\zeta(2a)\zeta(2b)\zeta(2c) + 2(2a-1)(2b-1)(2c-1)\zeta(2n) \right. \\
 & \left. - 3(2a-1)(2b-1)(2c-1)\zeta(2b)\zeta(2n-2b) \right\}. \tag{13.55}
 \end{aligned}$$

On the right hand side of (13.55), the sum for the first term can be taken care of by a small modification of (13.53); the sum for the second term is easy. The sum of the third term is slightly more troublesome; we first do the summation over indices a and c to obtain a single sum in b , let us denote it by $\sum_{b=2}^{n-2} S(n, b)$.

S is not symmetric, that is, $S(n, b) \neq S(n, n-b)$. We apply the trick of replacing S by $(S(n, b) + S(n, n-b))/2$. This symmetrises the summand so we may write it in closed form using Ramanujan’s identities (13.30) and (13.32). The final computation involves combining the closed forms obtained for the three terms in (13.55); the work is tedious though not difficult. \square

Remark 13.5.1. In [85], Dilcher works out a closed form for all sums of the type

$$\sum \binom{2n}{2a_1, 2a_2, \dots, 2a_k} B_{2a_1} B_{2a_2} \cdots B_{2a_k},$$

and notes the connection between this and sums of multiple zeta values (as early as 1994). Corresponding sums for Bernoulli polynomials are also recorded; indeed, using [85, eqn. (3.8)] with $x = 1/2, y = z = 0$, we get

$$\begin{aligned}
 \sum_{a+b+c=n} (4^{-a} + 4^{-b} + 4^{-c}) \zeta(2a, 2b, 2c) &= \frac{4^{-n}}{72} (7 \cdot 4^n + 128 + 141n - 18n^2) \zeta(2n) \\
 - \frac{3(1 + 2^{3-2n})}{16} \zeta(2) \zeta(2n-2) &+ \frac{1}{2} \sum_{i=1}^{n-1} 4^{-i} i \zeta(2i) \zeta(2n-2i), \tag{13.56}
 \end{aligned}$$

unfortunately the last sum does not appear to have a closed form, as strongly suggested by numerical experimentation (see the proof of Lemma 13.2). \diamond

Using the result for the sum of product of 5 Bernoulli numbers, and aided by the stuffle product, we deduce the next result much the same way as its length 3 or 4 analog in [67]:

Theorem 13.7. For integer $n \geq 5$,

$$\sum_{a+b+c+d+e=n} \zeta(2a, 2b, 2c, 2d, 2e) = \frac{945}{16} \zeta(2n) - \frac{315}{8} \zeta(2) \zeta(2n-2) + \frac{45}{8} \zeta(4) \zeta(2n-4). \quad (13.57)$$

SKETCH OF PROOF. We start with the length 5 analog of (13.47), obtainable using the stuffle product, which writes $\zeta(2a)\zeta(2b)\zeta(2c)\zeta(2d)\zeta(2e)$ as a symmetric sum of multiple zeta values of lengths no greater than 5. As stated, we use the sum of the product of 5 Bernoulli numbers [85, eqn. (2.8)], both of Ramanujan's identities (13.30), (13.32), and the length 3 and 4 sums (13.48) and (13.51). The key steps are spelled out in the proof of (13.54). In addition, only one more sum, (13.58) below, is required. This sum must have been known, but we are unable to locate it in the literature. We prove (13.58) next. \square

Lemma 13.2. For integer $n \geq 3$,

$$\sum_{\substack{a+b+c=n \\ a,b,c>0}} abc \zeta(2a)\zeta(2b)\zeta(2c) = \frac{3(2n-5)}{2} \zeta(4)\zeta(2n-4) + \frac{(2n-1)(2n-2)(2n-6)}{32} \times \\ \zeta(2)\zeta(2n-2) + \frac{(2n+2)(2n+1)(2n)(2n-1)(2n-2)}{3840} \zeta(2n). \quad (13.58)$$

PROOF. We again stress that the proof is not difficult once the result is known. Indeed, the left hand side is the coefficient of the cube of the generating function for jB_{2j} , and the right hand side is the coefficient of a combination of derivatives of the generating function for B_{2j} . The more interesting part is how this identity was discovered.

It was discovered *experimentally* after we were convinced that a closed form like Theorem 13.7 must exist. Then, it was easy to guess that the right hand side of Theorem 13.7 has the form

$$a_0 \zeta(2n) + a_1 \zeta(2) \zeta(2n-2) + a_2 \zeta(4) \zeta(2n-4),$$

c. f. the length 4 analog (13.51). The coefficients a_i can be solved by evaluating the left hand side to high precision for three different n 's. From this knowledge we can work backwards and discover the lemma. High precision calculation of multiple zeta values can be accessed from the website <http://oldweb.cecm.sfu.ca/projects/EZFace/>, based on the works [49, 50].

Alternatively, inspired by Ramanujan’s identities, one could reasonably guess that the right hand side of (13.58) would look something like

$$p_0(n)\zeta(2n) + p_1(n)\zeta(2)\zeta(2n - 2) + p_2(n)\zeta(4)\zeta(2n - 4),$$

where p_i are polynomials in n of degree say at most 5. The unknown coefficients in the polynomials then may be solved by linear algebra, since the left hand side of (13.58) can be computed very easily for small n . □

Lemma 13.2 itself leads to a different result, which is another three dimensional analogue of (13.31):

Proposition 13.5. *For integer $n \geq 3$,*

$$\sum_{a+b+c=n} abc \zeta(2a, 2b, 2c) = \frac{16(2n - 5)\zeta(4)\zeta(2n - 4) - 4\zeta(2)\zeta(2n - 2) + n\zeta(2n)}{128}. \tag{13.59}$$

Although it appears that equation (13.58) could follow from equations (13.46) and (13.53), we have not been able to see a clear connection; indeed, all three equations can be used together to deduce

$$\begin{aligned} & \sum_{\substack{a+b+c=n \\ a,b,c>0}} (a^2 + b^2 + c^2) \zeta(2a)\zeta(2b)\zeta(2c) \\ &= \frac{n(n + 1)(2n + 1)^2}{16} \zeta(2n) - \frac{(3n - 3)(4n - 3)}{4} \zeta(2)\zeta(2n - 2). \end{aligned}$$

Remark 13.5.2. Note that the right hand side of Theorem 13.7 is a rational multiple of π^{2n} , and the same is true for (13.51) and (13.48). Though it is not immediately clear to us whether for length k , there exists analogous closed forms like Theorem 13.7, it is not hard to show that for all positive integers $k \leq n$ and $a_i > 0$,

$$\sum_{a_1+a_2+\dots+a_k=n} \zeta(2a_1, 2a_2, \dots, 2a_k) = C_{k,n} \pi^{2n}, \quad C_{k,n} \in \mathbb{Q}. \tag{13.60}$$

The proof essentially involves repeated applications of the stuffle product $*$, for whose properties we refer the reader to [115]. In particular, $*$ is commutative and associative. A brief sketch is as follows.

The key observation, which can be proven by induction, is that the stuffle product $s_1 * s_2 * \dots * s_k$ generates the identity

$$\zeta(s_1)\zeta(s_2)\cdots\zeta(s_k) = \sum \zeta(s_1 \circ s_2 \circ \dots \circ s_k), \tag{13.61}$$

where \circ has to be one of ‘,’ or ‘+’, and the summation range is over *all possible* distinct sequences $(s_1 \circ s_2 \circ \dots \circ s_k)$ ($(s_1, s_2 + s_3)$ and $(s_1 + s_2, s_3)$ are distinct, but the first one and $(s_1, s_3 + s_2)$ are not). For $k = 3$, see (13.47) (where we have replaced pairs of double zeta values using (13.2)).

The next step is to systematically subtract off from the right hand side of (13.61) the symmetric sum (modulo commutativity and associativity) of identities generated by the stuffle product $s_1 \odot s_2 \odot \dots \odot s_k$. Here \odot has to be one of $*$ or $+$, moreover the operator $+$ takes precedence over $*$. To do this properly, we need to first subtract off the identities with only one $+$, then ones with only two $+$'s, etc. (So for $k = 3$, we first subtract off the identities generated by $s_1 + s_2 * s_3$, $s_1 + s_3 * s_2$, $s_2 * s_3 + s_1$, then $s_1 + s_2 + s_3$). It can be checked, using a form of (13.61) with different values of s_i substituted, that this process will terminate, and on the right hand side of (13.61) will only remain a symmetric sum of length k multiple zeta values with parameters s_1, \dots, s_k . On the other side will be a sum of products of zeta values, whose arguments sum to $s_1 + \dots + s_k$.

Finally, let $s_i = 2a_i$, fix $s_1 + \dots + s_k = 2n$ and sum over all a_i , we arrive at (13.60).

Independent of us, this result seems to have been first proven by S. Muneta. We thank Y. Ohno and W. Zudilin for communicating this information. \diamond

13.6. Another proof of Zagier's identity

D. Zagier recently proved the amazing multiple zeta formula [201]

$$\zeta(\underbrace{2, \dots, 2}_a, 3, \underbrace{2, \dots, 2}_b) = \sum_{r=1}^{a+b+1} (-1)^r \left[\left(1 - \frac{1}{4^r}\right) \binom{2r}{2a+1} - \binom{2r}{2b+2} \right] \frac{2\pi^{2(a+b-r+1)}\zeta(2r+1)}{(2(a+b-r+1)+1)!}. \tag{13.62}$$

His proof in [201] is rather involved. In this section we outline a simplification of the proof, showing in particular that some of the key identities involved can

be checked automatically using Gosper’s algorithm [161]. We refer the interested reader to [201] for the background of the formula and other details of the proof.

We first convert (13.62) to the equivalent form

$$\begin{aligned} & \zeta(\{2\}^m, 3, \{2\}^n) \\ = & 2 \sum_{r=1}^{m+n+1} (-1)^{r-1} \left(\left(1 - \frac{1}{2^{2r}}\right) \binom{2r}{2m+1} - \binom{2r}{2n+2} \right) \zeta(\{2\}^{m+n-r+1}) \zeta(2r+1), \end{aligned} \tag{13.63}$$

where $\{k\}^m$ means the argument k is repeated m times. The proof is completed in the following 6 steps.

1. It is not hard to check that the two-variable generating function of the left hand side of (13.63) is

$$\begin{aligned} F(x, y) &= \sum_{m, n \geq 0} (-1)^{m+n+1} \zeta(\{2\}^m, 3, \{2\}^n) x^{2m+1} y^{2n+2} \\ &= -xy^2 \sum_{r=1}^{\infty} \prod_{k=1}^{r-1} \left(1 - \frac{y^2}{k^2}\right) \cdot \frac{1}{r^3} \cdot \prod_{l=r+1}^{\infty} \left(1 - \frac{x^2}{l^2}\right) \\ &= \frac{\sin \pi x}{\pi} \frac{\partial}{\partial z} {}_3F_2 \left(\begin{matrix} y, -y, z \\ 1+x, 1-x \end{matrix} \middle| 1 \right) \Big|_{z=0} \\ &= \frac{\sin \pi x}{\pi} \sum_{r=1}^{\infty} \frac{(-y)_r (y)_r}{(-x+1)_r (x+1)_r} \frac{1}{r}. \end{aligned} \tag{13.64}$$

2. The generating function of the right hand side of (13.63) equals

$$\begin{aligned} \widehat{F}(x, y) &= 2 \sum_{m, n \geq 0} (-1)^{m+n} x^{2m+1} y^{2n+2} \sum_{r=1}^{m+n+1} (-1)^r \left((1 - 2^{-2r}) \binom{2r}{2m+1} \right. \\ & \quad \left. - \binom{2r}{2n+2} \right) \frac{\pi^{2(m+n-r+1)}}{(2(m+n-r+1)+1)!} \zeta(2r+1) \\ &= \frac{\sin \pi x}{\pi} (A(x+y) + A(x-y) - 2A(x)) - \frac{\sin \pi y}{\pi} (B(x+y) - B(x-y)), \end{aligned}$$

after some manipulations, where

$$A(t) = -\gamma - \frac{1}{2} (\Psi(1+t) + \Psi(1-t)) \quad \text{and} \quad B(t) = A(t) - A\left(\frac{t}{2}\right).$$

As usual, Ψ denotes the digamma function (see (5.24)).

3. Both $F(x, y)$ and $\widehat{F}(x, y)$ are entire functions on \mathbb{C}^2 . By standard estimates, it can be shown that for a fixed $x \in \mathbb{C}$, each of them is of exponential type and is

$O(e^{\frac{3}{2}\pi|y|})$ and $|y| \rightarrow \infty$. (In fact a much stronger estimate is possible, but we do not need it.)

4. For $x \in \mathbb{C}$, it is easy to check that

$$F(x, x) = -\frac{\sin \pi x}{\pi} A(x) = \widehat{F}(x, x),$$

and

$$F(x, 0) = 0 = \widehat{F}(x, 0).$$

The first 4 steps basically follow [201]. The goal is to show the sum in step 1 equals the digamma expression in step 2. Our next two steps replace the delicate analysis, including a technical result on two-variable entire functions, used in [201].

5. For each $x \in \mathbb{C}$, the function $f(x, y) := F(x, y) - \widehat{F}(x, y)$ is 1-periodic in y .

PROOF. Note that

$$(z)_r(y+1)_r - (z+1)_r(y)_r = (z)_r(y)_r \cdot r \left(\frac{1}{y} - \frac{1}{z} \right).$$

Therefore, choosing $z = -y - 1$, we obtain

$$F(x, y+1) - F(x, y) = \frac{\sin \pi x}{\pi} \frac{2y+1}{y(y+1)} \sum_{r=1}^{\infty} \frac{(-y-1)_r(y)_r}{(-x+1)_r(x+1)_r}.$$

The latter hypergeometric sum is Gosper-summable: if we take

$$\Lambda(r) = \frac{x^2 - y(y+1) + r}{(x-y)(x+y)(x-y-1)(x+y+1)} \cdot \frac{(-y-1)_{r+1}(y)_{r+1}}{(-x+1)_r(x+1)_r},$$

then

$$\Lambda(r) - \Lambda(r-1) = \frac{(-y-1)_r(y)_r}{(-x+1)_r(x+1)_r}.$$

Furthermore,

$$\begin{aligned} \frac{(-y-1)_{r+1}(y)_{r+1}}{(-x+1)_r(x+1)_r} &= -xy(y+1) \cdot \frac{\Gamma(x-r)\Gamma(y+r+1)}{\Gamma(x+r+1)\Gamma(y-r+1)} \\ &= xy(y+1) \frac{\sin \pi y}{\sin \pi x} \frac{\Gamma(r-y)\Gamma(r+y+1)}{\Gamma(r-x+1)\Gamma(r+x+1)} \\ &\sim xy(y+1) \frac{\sin \pi y}{\sin \pi x} \left(\frac{(1 - \frac{y+1}{r})(1 + \frac{y}{r})}{(1 - \frac{x}{r})(1 + \frac{x}{r})} \right)^r \frac{e}{r} \\ &\sim xy(y+1) \frac{\sin \pi y}{\sin \pi x} \frac{1}{r} \quad \text{as } r \rightarrow \infty. \end{aligned}$$

Thus,

$$\begin{aligned} F(x, y+1) - F(x, y) &= \frac{\sin \pi x}{\pi} \frac{2y+1}{y(y+1)} (\Lambda(\infty) - \Lambda(0)) \\ &= \frac{\sin \pi y}{\pi} \frac{x(2y+1)}{(x-y)(x+y)(x-y-1)(x+y+1)} \\ &\quad + \frac{\sin \pi x}{\pi} \frac{(x^2 - y(y+1))(2y+1)}{(x-y)(x+y)(x-y-1)(x+y+1)}. \end{aligned}$$

A routine verification shows that a similar result holds for $\widehat{F}(x, y+1) - \widehat{F}(x, y)$.

This implies the desired 1-periodicity. \square

6. For each $x \in \mathbb{C} \setminus \mathbb{Z}$, the function $f(x, y)$ is zero, so that it vanishes for all $x, y \in \mathbb{C}$, implying $F(x, y) = \widehat{F}(x, y)$.

PROOF. We fix an arbitrary $x \notin \mathbb{Z}$. It follows from steps **3–5** that the entire 1-periodic function $f(x, y)$ vanishes at $y = x$ and $y = 0$. Therefore,

$$g(y) := \frac{f(x, y)}{\sin \pi(y-x)}$$

is an entire function of exponential type, which vanishes at the integers and whose growth is $O(e^{\frac{1}{2}\pi|y|})$ on the imaginary axis. Therefore, by Carlson's Theorem **1.3**, $g(y)$ vanishes identically, and so does $f(x, y)$. \square

Remark 13.6.1. Zagier [**201**] asks if a hypergeometric proof of (13.62) could be found. The paper [**135**] answers the question in the affirmative. The first step involves transforming the ${}_3F_2$ in (13.64) twice (curiously, one of the transformations is also used in Remark 7.10.1), so that in the resulting ${}_3F_2$, the derivative with respect to parameter z at 0 is particularly simple. In fact, in the derivative, some terms vanish while the remaining ones evaluate in terms of Ψ by a formula in [**131**] (such formulas are not uncommon, see e.g. Theorem 5.5). The Ψ expression obtained simplifies to the required terms in step **2**. \diamond

Further Applications of Experimental Mathematics

ABSTRACT. In this chapter we deal with two applications of experimental mathematics. The first section addresses the problem of finding, proving and simplifying contiguous relations, with help from PSLQ. The next two sections outline a method to discover and investigate orthogonal polynomials starting with Gram-Schmidt orthogonalisation, with an application in Gaussian quadrature to approximate a range of sums.

14.1. Contiguous relations

When the matching parameters in two generalised hypergeometric functions with the same argument differ by integers, they are said to be *contiguous* [11]. For instance,

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| x\right) \quad \text{and} \quad {}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{3}{2} \\ 1, 2 \end{matrix} \middle| x\right)$$

are contiguous. (In the terminology of [179], such a pair is called *associated*, while the term *contiguous* is reserved for the case when only one pair of parameters differ, and only by unity. We do not make this distinction here.)

It was Gauss who showed that a ${}_2F_1$ can be written as a linear combination of any two of its contiguous functions, with rational coefficients in terms of the parameters and the argument. Such combinations, known as contiguous relations, are of importance in dealing with hypergeometric sums, and feature in many results from Chapters 3, 5, 6, 7 and 12. There is a large but scattered literature on contiguous relations, see for example [11, 27, 162, 198, 122]. We hope to present a slightly more unified treatment here.

14.1.1. Raising and lowering operators. We consider the hypergeometric function

$$F(a, a_1, \dots, a_n; b, b_1, \dots, b_{n-1}; x) = {}_{n+1}F_n\left(\begin{matrix} a, a_1, \dots, a_n \\ b, b_1, \dots, b_{n-1} \end{matrix} \middle| x\right).$$

(All the theory here also works for a general ${}_pF_q$, we simply find the stated function more useful.) When the function used is understood from the context, we simply denote it by F , or $F(a)$ to highlight the parameter of interest. We use $F(a+)$ to denote F with a replaced by $a + 1$; similar conventions hold for other parameters. We also use D to denote the operator with the effect that $DF = x \frac{dF}{dx}$. It follows from straightforward series manipulations that (for any valid set of parameters and n)

$$a F(a+) = (D + a)F, \quad (14.1)$$

$$(b - 1) F(b-) = (D + b - 1)F. \quad (14.2)$$

These two useful contiguous relations allow us to raise a ‘top’ parameter by 1, and to lower a ‘bottom’ parameter by 1. In order to lower the top by 1 or to raise the bottom by 1, we need to resort to the hypergeometric *differential equation*:

$$[D(D + b - 1)(D + b_1 - 1) \cdots (D + b_{n-1} - 1) - x(D + a)(D + a_1) \cdots (D + a_n)]F = 0. \quad (14.3)$$

In (14.3), replacing a by $a - 1$ and factoring out $D + a - 1$ (which can be achieved by formally setting $D = 1 - a$), we have

$$(a - 1)(b - a)(b_1 - a) \cdots (b_{n-1} - a)F(a-) = \Delta_1(D - a - 1)F(a-),$$

where Δ_1 is a differential operator involving only the parameters, x , and powers of D . Replacing the last two terms on the right by (14.1) (again with $a \mapsto a - 1$), we obtain a formula for $F(a-)$.

Similarly, in (14.3), replacing b by $b + 1$ and factoring out $D + b$ gives

$$x(a - b)(a_1 - b) \cdots (a_n - b)F(b+) = \Delta_2(D + b)F(b+),$$

where Δ_2 is similar in nature to Δ_1 . Invoking (14.2), we obtain a formula for $F(b+)$. The form for a ${}_3F_2$ is recorded in (14.6).

In summary, the operators $F(a\pm)$ and $F(b\pm)$ exist and are very easily computable with a computer algebra system. The formulas for $F(a-)$ and $F(b+)$ only involve the functions $x^i F, x^i DF, \dots, x^i D^n F$ for $i \in \{-1, 0, 1\}$. Moreover, when $x = 1$, we see that in (14.3) the D^n term disappears and hence cannot appear in the contiguous relations. (In practice, expressions of $D^n F$ may involve $x - 1$ in

the denominator, so at $x = 1$ it may need to be simplified using L'Hôpital's rule.) Armed with the four raising and lowering operators, we have:

Theorem 14.1. *Any function contiguous to F can be expressed in terms of $F, DF, \dots, D^{n-1}F, D^n F$, and a contiguous relation may be obtained from any $n+2$ contiguous functions (by means of elimination). When $x = 1$, the $D^n F$ term is not required and we only need $n+1$ functions.*

Theorem 14.1 was essentially known to Bailey [27], who comments that “It would be a very tedious process to obtain some of these results directly by the general method of this paper” (pertaining to finding contiguous functions from the four operators). With the advent of computer algebra systems, we see that this is no longer the case, for such operations can be quickly and faithfully carried out on even a modest machine. Moreover, in the next section we present another method of obtaining contiguous functions.

Remark 14.1.1. The following contiguous relations are easy to prove and are occasionally useful:

$$\begin{aligned}(a - a_i)F &= aF(a+) - a_iF(a_i+), \\ (a - b + 1)F &= aF(a+) - (b - 1)F(b-), \\ (b - b_i)F &= (b - 1)F(b-) - (b_i - 1)F(b_i-).\end{aligned}\tag{14.4}$$

◇

14.1.2. PSLQ and contiguous functions. We start with an example.

Example 14.1.1. Suppose F is a ${}_3F_2$ and we want a contiguous relation in terms of $F(a), F(a+1), F(a+2), F(a+3)$; such a relation is guaranteed to exist by Theorem 14.1. Instead of using the four operators $F(a\pm)$ and $F(b\pm)$, we realise that equation (14.3) indicates F can be written as a linear combination of $x^i D^j F$, where $i \in \{0, 1\}$ and $j \in \{1, 2, 3\}$. Using (14.1) repeatedly, we see that these terms simplify into the form $(u_k + v_k x)F(a+k)$ for $k \in \{0, 1, 2, 3\}$ for some u_k and v_k , and the power of x involved is at most 1. That is, we have

$$\sum_{k=0}^3 (u_k + v_k x)F(a+k) = 0.\tag{14.5}$$

We expand the ${}_3F_2$'s in (14.5) as sums in n , extract the summands of x^n and simplify, then solve for u_k, v_k . This can be done by substituting in values of the summation variable to form enough equations (here we need 8); or by collecting the expression into a single fraction, and setting up a system of linear equations with the aim of making the numerator disappear identically. Either way we obtain the desired contiguous relation (with humongous coefficients).

Specialising the relation by setting $a = 0, x = 1$, for instance, and we get

$$\begin{aligned} & ((2-d)(2-e) - (1-b)(1-c)) {}_3F_2\left(\begin{matrix} 1, b, c \\ d, e \end{matrix} \middle| 1\right) \\ & = (2+b+c-d-e) {}_3F_2\left(\begin{matrix} 2, b, c \\ d, e \end{matrix} \middle| 1\right) + (1-d)(1-e). \end{aligned}$$

◇

There are a few observations about the above derivation. Firstly it works for a general ${}_pF_q$, and for contiguous relations of any desired form. Secondly, for other forms of relations, it is conceivable that we may not be so lucky as to only get linear powers of x , so we may need to enter higher powers of x in the equivalent of (14.5) in search of a relation. Note that this ‘guess, simplify and solve’ routine is similar to Celine’s algorithm [161].

How do we know which powers of x to use? This is when the integer relation program PSLQ comes in. We have the following **procedure**:

Suppose we want to find a relation between some hypergeometric functions F_i . Pick the parameters to be *rational* and pick a small, *irrational* x . Compute, to high precision (which is possible as x is small), $x^j F_i$ for $j = -J_0, \dots, -1, 0, 1, \dots, J_1$ where J_0, J_1 are appropriate integers. Run PSLQ on these constants; if no relation is found, increase J_0, J_1 . If a relation is found, then the equivalent form of (14.5) is very likely to involve the non-zero terms in the relation (since the irrationality of x minimises the likelihood of spurious relations). We then extract the summand, simplify and solve for the coefficients, as we did for (14.5). Once a solution is found, the corresponding relation is proven.

Example 14.1.2. For instance, let us find $F = {}_3F_2(a-1, b-1, c; d+1, e; x)$ in terms the F_i , the i th derivatives of ${}_3F_2(a, b, c; d, e; x)$, without using the operators $F(a\pm)$ and $F(b\pm)$ (which would require 3 applications).

We pick $J_0 = 0, J_1 = 3$, and run PSLQ on the vector with elements F and $x^j F_i$ with $i \in \{0, 1, 2\}$, for appropriately chosen parameters and x . A relation is found, and so we have discovered that

$$F = (u_1 + u_2x)F_0 + (u_3 + u_4x + u_5x^2)F_1 + x(u_6 + u_7x + u_8x^2)F_2,$$

for some u_1, \dots, u_8 . We can extract the summand and solve for the u_j , which are rather complicated functions of the parameters. \diamond

Example 14.1.3. An important application of examples like 14.1.2 is the evaluation of hypergeometric functions in terms of other functions. If F is expressible in terms of well-known functions, then we can write any function contiguous to F in terms of F and its derivatives. For instance, since

$${}_3F_2\left(\begin{matrix} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{matrix} \middle| x\right) = \frac{4}{\pi^2} K^2\left(\sqrt{\frac{1 - \sqrt{1-x}}{2}}\right),$$

Example 14.1.2 gives, after some simplification,

$$\begin{aligned} \frac{9\pi^2 t^2(1-t^2)}{4} {}_3F_2\left(\begin{matrix} -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2} \\ 1, 2 \end{matrix} \middle| 4t^2(1-t^2)\right) &= (t^2 - 1)(12t^4 - 22t^2 + 1)K^2(t) \\ &- 2(t^2 - 1)(12t^4 - 26t^2 + 1)E(t)K(t) - (40t^4 - 40t^2 + 1)E^2(t). \end{aligned}$$

Computations like this form the basis of the contiguous relations required in Chapter 12. \diamond

The raising and lowering operators can also be written in terms of the F' (instead of ΔF), and we record here that for $F := {}_3F_2(a, b, c; d, e; x)$,

$$\begin{aligned} F(a-) &= \left[1 - \frac{bcx}{(a-d)(a-e)}\right]F - \frac{a-d-e+(1+b+c)x}{(a-d)(a-e)}x F' + \frac{x^2(1-x)F''}{(a-d)(a-e)}, \\ F(d+) &= \left[1 - \frac{abc}{(a-d)(b-d)(c-d)}\right]F + \frac{e-(1+a+b+c-d)x}{(a-d)(b-d)(c-d)/d}F' \\ &+ \frac{dx(1-x)F''}{(a-d)(b-d)(c-d)}. \end{aligned} \tag{14.6}$$

Remark 14.1.2. In Chapter 3, the proof of lemma 3.1 uses the raising operator (14.6) repeatedly to obtain a differential expression which simplifies to 0. This seems to be a powerful and previously unexploited method to prove a wide range of contiguous relations with fixed arguments.

In Chapter 7, in order to work out a number of incomplete moments, we needed a closed form expression for ${}_3F_2(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; 1, 2; t)$; this can be easily done using (14.6).

We also note that contiguous relations with (free) argument x are generally easy to prove, once discovered, by looking at the series expansion; relations with argument 1 can often be proven using Gosper's algorithm [161], as we did several times in Chapter 6. \diamond

14.1.3. Contiguous summation formulas. Many exact summation formulas in terms of Γ functions are available for certain special hypergeometric functions (as we saw in some $1/\pi$ evaluations in Chapters 10 and 12). Almost always, such formulas are stated in the literature in their cleanest and simplest forms, however in many cases functions contiguous to the stated ones also possess closed forms. In particular, these contiguous closed form summation formulas are not handled automatically in computer algebra systems. We collect some results here.

Kummer's theorem. Kummer's theorem [25] evaluates certain ${}_2F_1$'s at -1 :

$${}_2F_1\left(\begin{matrix} a, b \\ 1 + a - b \end{matrix} \middle| -1\right) = \frac{\Gamma(1 + a - b)\Gamma(1 + \frac{a}{2})}{\Gamma(1 + \frac{a}{2} - b)\Gamma(1 + a)}. \quad (14.7)$$

However, there is actually a closed form formula for ${}_2F_1(a, b; n + a - b; -1)$ for all integer n . When $n \geq 1$, we use the Euler integral (4.3) to write the ${}_2F_1$ as

$$\frac{\Gamma(n + a - b)}{\Gamma(a)\Gamma(n - b)} \int_0^1 x^{a-1}(1-x^2)^{-b}(1-x)^{n-1} dx,$$

so we can expand out the last factor binomially and apply the beta integral to each term; therefore

$${}_2F_1\left(\begin{matrix} a, b \\ 1 + n + a - b \end{matrix} \middle| -1\right) = \frac{\Gamma(1 - b)\Gamma(n + 1 - b + a)}{2\Gamma(a)\Gamma(n + 1 - b)} \sum_{k=0}^n \frac{(-1)^k \binom{n}{k} \Gamma(\frac{a+k}{2})}{\Gamma(1 - b + \frac{a+k}{2})}. \quad (14.8)$$

When b is a positive integer, this formula is to be understood in the limiting sense, first fixing n . Similarly, we also have

$${}_2F_1\left(\begin{matrix} a, b \\ 1 - n + a - b \end{matrix} \middle| -1\right) = \frac{\Gamma(1 + a - b - n)}{2\Gamma(a)} \sum_{k=0}^n \frac{\binom{n}{k} \Gamma(\frac{a+k}{2})}{\Gamma(1 - b - n + \frac{a+k}{2})}. \quad (14.9)$$

For fixed n , these formulas can collapse down naturally into two terms due to the Γ recursion. In particular, when $n = 1$, the formula is rather succinct:

$${}_2F_1\left(\begin{matrix} a, b \\ a - b \end{matrix} \middle| -1\right) = \frac{\Gamma(a - b)}{2\Gamma(a)} \left[\frac{\Gamma(\frac{a}{2})}{\Gamma(\frac{a}{2} - b)} + \frac{\Gamma(\frac{a+1}{2})}{\Gamma(\frac{a+1}{2} - b)} \right].$$

Gauss's second theorem and Bailey's theorem. These theorems give closed form evaluations of certain ${}_2F_1$'s at $1/2$ [25]; one obvious application is in the

computation of the value of $K(1/\sqrt{2})$ which we have used many times, another is seen in Section 10.8. Using Euler’s transformation (6.32) (mapping $z \mapsto z/(z-1)$), equations (14.8) and (14.9) imply that both

$${}_2F_1\left(\begin{matrix} a, b \\ \frac{n+a+b}{2} \end{matrix} \middle| \frac{1}{2}\right) \quad \text{and} \quad {}_2F_1\left(\begin{matrix} a, n-a \\ c \end{matrix} \middle| \frac{1}{2}\right)$$

have closed forms in terms of Γ functions for all integer n . Some special cases of (14.8) and (14.9) have been found in [163].

Saalschütz’s theorem. This theorem for a terminating ${}_3F_2$ is traditionally stated as [25]

$${}_3F_2\left(\begin{matrix} a, b, -n \\ c, 1+a+b-c-n \end{matrix} \middle| 1\right) = \frac{(c-a)_n(c-b)_n}{(c)_n(c-a-b)_n}, \tag{14.10}$$

where n is a non-negative integer. We can generalise (14.10) here. It is not hard to see that the coefficient of z^n in

$$(1-z)^{m-1} {}_2F_1\left(\begin{matrix} c-a, c-b \\ c \end{matrix} \middle| z\right) \tag{14.11}$$

is

$$\binom{c-a-b-m+n}{n} {}_3F_2\left(\begin{matrix} a, b, -n \\ c, m+a+b-c-n \end{matrix} \middle| 1\right),$$

and when $m \geq 1$ is an integer it is routine to extract the coefficient of z^n in (14.11).

For instance, when $m = 2$,

$$\begin{aligned} {}_3F_2\left(\begin{matrix} a, b, -n \\ c, 2+a+b-c-n \end{matrix} \middle| 1\right) = & \tag{14.12} \\ \frac{(c-a)_n(c-b)_n}{(c)_n(c-a-b)_n} \left[1 - \frac{abn}{(1+a+b-c)(1+a-c-n)(1+b-c-n)} \right]. \end{aligned}$$

Note that closed forms are unlikely for $m < 1$: even when $m = 0$, the coefficients are the partial sums of the ${}_2F_1$, so Gosper’s algorithm indicates there is no universal closed form. However, in the $m = 0$ case we can often find ad-hoc solutions (e. g. in terms of harmonic numbers) by entering special values of a, b and c .

The paper [121] considers the $m = 2$ and 3 cases based on applying (6.32) on the beta integral for (14.10).

We note that when the (14.11) is written as a convolution sum, the generalisation of Saalschütz’s theorem is just the transformation below; when $m \geq 1$ is integral

and fixed the right hand side can thus be evaluated:

$${}_3F_2\left(\begin{matrix} a, b, -n \\ c, m+a+b-c-n \end{matrix} \middle| 1\right) = \frac{(c-a)_n(c-b)_n}{(c)_n(c-a-b+1-m)_n} \\ \times {}_3F_2\left(\begin{matrix} 1-m, 1-c-n, -n \\ 1+a-c-n, 1+b-c-n \end{matrix} \middle| 1\right). \quad (14.13)$$

Dixon's theorem. Dixon's theorem [25] is the main tool for evaluating non-terminating ${}_3F_2$'s at 1. (Other tools include Clausen's formula and Orr-type theorems, which rely on a factorisation of the ${}_3F_2$ – see Chapter 12; also see the Watson's and Whipple's theorems below.) The theorem states that

$${}_3F_2\left(\begin{matrix} a, b, c \\ 1+a-b, 1+a-c \end{matrix} \middle| 1\right) = \frac{\Gamma(1+\frac{a}{2})\Gamma(1+a-b)\Gamma(1+a-c)\Gamma(1+\frac{a}{2}-b-c)}{\Gamma(1+a)\Gamma(1+\frac{a}{2}-b)\Gamma(1+\frac{a}{2}-c)\Gamma(1+a-b-c)}, \quad (14.14)$$

and a very special case is the celebrated identity,

$$\sum_{k=0}^{2n} \binom{2n}{k}^3 (-1)^{k+n} = \frac{(3n)!}{n!^3}.$$

Lavoie et. al [131] have given contiguous evaluations of Dixon's theorem – the results are beautifully presented there, so we do not reproduce them. Independently, we show how such results may be achieved. Denote the generic function ${}_3F_2(a, b, c; d, e; 1)$ by F , and let

$$F_{m,n} := {}_3F_2\left(\begin{matrix} a, b, c \\ m+a-b, n+a-c \end{matrix} \middle| 1\right). \quad (14.15)$$

Dixon's theorem is a closed form for $F_{1,1}$; also note the symmetry in m and n . Our result is the following:

Theorem 14.2. *There exists closed forms for $F_{m,n}$, where m and n are integers that satisfy $0 \leq m \leq n \leq 2$.*

PROOF. Let $\tilde{F} = F_{2,2}$. Our first strategy is to note that $\tilde{F}(a+)$ and $\tilde{F}(d-, e-)$ can both be evaluated using the classical version of Dixon's theorem (14.14). By Theorem 14.1, there exists a contiguous relation between \tilde{F} , $\tilde{F}(a+)$ and $\tilde{F}(d-, e-)$. Indeed, the last two terms may be related to \tilde{F} and its derivatives using the raising and lowering operators; aided by the differential equation (14.3) at 1, we arrive at

$$(d-1)(e-1)\tilde{F}(d-, e-) - a\left(d+e-1 - \frac{(1+b)(1+c) + a(1+b+c) - de}{2+a+b+c-d-e}\right)\tilde{F}(a+) \\ - \frac{(1+a-d)(1+a-e)(2+b+c-d-e)}{2+a+b+c-d-e}\tilde{F} = 0.$$

This leads to

$$F_{2,2} = \frac{2^{1-2c} \Gamma(2+a-b)\Gamma(2+a-c)}{(b-1)(c-1)\Gamma(2+a-2c)\Gamma(2+a-b-c)} \\ \times \left[\frac{\Gamma(\frac{3+a-2c}{2})\Gamma(\frac{4+a-2b-2c}{2})}{\Gamma(\frac{1+a}{2})\Gamma(\frac{2+a-2b}{2})} - \frac{\Gamma(\frac{2+a-2c}{2})\Gamma(\frac{5+a-2b-2c}{2})}{\Gamma(\frac{a}{2})\Gamma(\frac{3+a-2b}{2})} \right]. \quad (14.16)$$

For $F_{1,2}$, we simply find a contiguous relation between $F_{1,2}$, $F_{1,2}(e-)$ and $F_{1,2}(a+, b+)$, noting that the last two can be evaluated using Dixon's theorem. The result is

$$F_{1,2} = \frac{2^{-a} \sqrt{\pi} \Gamma(1+a-b)\Gamma(2+a-c)}{(c-1)\Gamma(2+a-b-c)} \\ \times \left[\frac{\Gamma(\frac{3+a-2b-2c}{2})}{\Gamma(\frac{a}{2})\Gamma(\frac{1+a-2b}{2})\Gamma(\frac{3+a-2c}{2})} - \frac{\Gamma(\frac{4+a-2b-2c}{2})}{\Gamma(\frac{1+a}{2})\Gamma(\frac{2+a-2b}{2})\Gamma(\frac{2+a-2c}{2})} \right]. \quad (14.17)$$

For $F_{0,1}$, we just find a contiguous relation between $F_{0,1}$, $F_{0,1}(b+)$ and $F_{0,1}(a-, e-)$, where the last two can be evaluated using Dixon's theorem. Note that there is a simpler contiguous relation between $F_{0,1}$, $F_{0,1}(b+)$ and $F_{0,1}(d+)$, but upon specialising the coefficients (so that the last two terms satisfy the conditions of Dixon's theorem), this relation collapses down to $0 = 0$ and is hence not helpful. The first contiguous relation gives

$$F_{0,1} = \frac{2^{-a} \sqrt{\pi} \Gamma(a-b)\Gamma(1+a-c)}{\Gamma(1+a-b-c)} \\ \times \left[\frac{\Gamma(\frac{1+a-2b-2c}{2})}{\Gamma(\frac{a}{2})\Gamma(\frac{1+a-2b}{2})\Gamma(\frac{1+a-2c}{2})} + \frac{\Gamma(\frac{2+a-2b-2c}{2})}{\Gamma(\frac{1+a}{2})\Gamma(\frac{a-2b}{2})\Gamma(\frac{2+a-2c}{2})} \right]. \quad (14.18)$$

For $F_{0,0}$, we find a contiguous relation between $F_{0,0}$, $F_{0,0}(a-)$ and $F_{0,0}(c+, d+)$, again the last two can be evaluated using Dixon's theorem. It follows that

$$F_{0,0} = \frac{2^{-a} \sqrt{\pi} \Gamma(a-b)\Gamma(a-c)}{\Gamma(a-b-c)} \\ \times \left[\frac{\Gamma(\frac{1+a-2b-2c}{2})}{\Gamma(\frac{a}{2})\Gamma(\frac{1+a-2b}{2})\Gamma(\frac{1+a-2c}{2})} + \frac{\Gamma(\frac{a-2b-2c}{2})}{\Gamma(\frac{1+a}{2})\Gamma(\frac{a-2b}{2})\Gamma(\frac{a-2c}{2})} \right]. \quad (14.19)$$

For $F_{0,2}$, many contiguous relations in which two of the terms can be evaluated using Dixon's theorem return $0 = 0$. Therefore we adopt a *second* strategy, using

contiguous relations and other known values of $F_{m,n}$; here the equations (14.4) come in handy. Indeed, the second equation in (14.4) gives

$$F_{0,2} = \frac{b}{b+c-a-1} F_{1,2}(b+) + \frac{c-a-1}{b+c-a-1} F_{0,1}. \quad (14.20)$$

Therefore we can read off $F_{0,2}$ from formulas for the right hand side already given. \square

Remark 14.1.3. A *third*, though tedious, way to find closed form expressions for $F_{m,n}$ is to imitate the proof of Dixon's theorem in [25].

In brief, we consider the infinite sum in the variable k for $F_{m,n}$, and factor out terms in the summand that are the evaluation of ${}_2F_1(b+k+m-1, c+k+n-1, a+2k+m+n-1, 1)$ by Gauss' theorem (5.3).

Writing these terms as a ${}_2F_1$, we then convert it into an infinite sum in j , let $p = j+k$ and change the order of summation in the resulting double sum. The sum in k in some cases decomposes into a number of ${}_2F_1$'s at -1 , which can be summed using contiguous versions of Kummer's theorem (14.8) and (14.9). Each piece, then summed in p , results in a ${}_2F_1$ with argument 1, this way we obtain our closed form. For instance, $F_{-1,0}$, $F_{0,0}$ and $F_{0,1}$ can be found in this manner.

Clearly, a combination of the three strategies presented here enables us to find closed forms for $F_{m,n}$ for many more pairs of m and n . \diamond

Watson's and Whipple's theorems. These theorems, recorded in [25], follow from Dixon's theorem and Thomae's transformation (see [25, p. 14]); they give, respectively, closed form evaluations for

$${}_3F_2\left(\begin{matrix} a, b, c \\ \frac{a+b+1}{2}, 2c \end{matrix} \middle| 1\right) \quad \text{and} \quad {}_3F_2\left(\begin{matrix} a, 1-a, c \\ e, 2c+1-e \end{matrix} \middle| 1\right).$$

Since we have results contiguous to Dixon's theorem, it follows that we can obtain many results related to Watson's and Whipple's theorems. They are cumbersome and we only list two here:

$${}_3F_2\left(\begin{matrix} a, b, c \\ \frac{a+b}{2}, 2c \end{matrix} \middle| 1\right) = \sqrt{\pi} \Gamma\left(\frac{a+b}{2}\right) \Gamma\left(\frac{1+2c}{2}\right) \Gamma\left(\frac{2c-a-b}{2}\right) \quad (14.21)$$

$$\begin{aligned} & \times \left[\frac{1}{\Gamma\left(\frac{a}{2}\right) \Gamma\left(\frac{1+b}{2}\right) \Gamma\left(\frac{2c-a}{2}\right) \Gamma\left(\frac{1+2c-b}{2}\right)} + \frac{1}{\Gamma\left(\frac{1+a}{2}\right) \Gamma\left(\frac{b}{2}\right) \Gamma\left(\frac{1+2c-a}{2}\right) \Gamma\left(\frac{2c-b}{2}\right)} \right], \\ {}_3F_2\left(\begin{matrix} a, -a, c \\ e, 2c-e \end{matrix} \middle| 1\right) &= \frac{\Gamma(2c-e)\Gamma(e)}{2\Gamma(2c+a-e)\Gamma(e-a)} \quad (14.22) \\ & \times \left[\frac{\Gamma\left(\frac{2c+a-e}{2}\right) \Gamma\left(\frac{e-a}{2}\right)}{\Gamma\left(\frac{2c-a-e}{2}\right) \Gamma\left(\frac{e+a}{2}\right)} + \frac{\Gamma\left(\frac{1+2c+a-e}{2}\right) \Gamma\left(\frac{1+e-a}{2}\right)}{\Gamma\left(\frac{1+2c-a-e}{2}\right) \Gamma\left(\frac{1+e+a}{2}\right)} \right]. \end{aligned}$$

Some similar results are found in [130] and [132].

14.2. Orthogonal polynomials

We start with some results from the classical theory of orthogonal polynomials [11, Ch. 5]. Under mild conditions, for a non-decreasing function $\alpha(x)$ with finite moments, there exists a sequence of polynomials $\{p_n(x)\}_{n=0}^\infty$ where p_n has degree n , such that they are orthogonal with respect to (weight) α :

$$\int_a^b p_m(x)p_n(x) d\alpha = h_n \delta_{mn}, \quad (14.23)$$

here δ_{mn} denotes the Kronecker delta, which is 1 when $m = n$ and 0 otherwise.

Every polynomial of degree n can be expressed uniquely as a linear combination of p_0, \dots, p_n . We may normalise the p_n so that they are monic, and it is not hard to show that they satisfy a three-term recurrence relation

$$p_{n+1} = (x - a_n)p_n(x) - b_n p_{n-1}(x), \quad (14.24)$$

moreover, $b_n = h_n/h_{n-1}$.

Conversely, if a set of polynomials is generated from a 3-term recurrence of the form (14.24), then Favard's theorem [184] states that it is orthogonal with respect to some α .

The n th polynomial $p_n(x)$ is in fact the characteristic equation of a tridiagonal matrix, so that the zeros of $p_n(x)$ are the eigenvalues of the $n \times n$ tridiagonal matrix with a_0, \dots, a_{n-1} on the diagonal, b_1, b_2, \dots, b_{n-1} on the upper off-diagonal, and 1's on the lower off-diagonal. The n zeros of $p_n(x)$ are simple and separate the $n + 1$ zeros of $p_{n+1}(x)$.

Examples of orthogonal polynomials include the Legendre and Chebyshev polynomials, which we have discussed in previous chapters (especially 10 – 12). For the Legendre polynomials P_n , in the notations of (14.23) we have $a = -b = 1$, $d\alpha = dx$, $h_n = 2/(2n + 1)$, and the recursion is

$$(n + 1)P_{n+1}(x) = (2n + 1)xP_n(x) - nP_{n-1}(x). \quad (14.25)$$

We are interested in the case when α is a discrete measure, that is, the polynomials are orthogonal with respect to *summation* instead of integration:

$$\sum_x p_m(x)p_n(x)\alpha(x) = h_n\delta_{mn}.$$

When such polynomials can be represented by hypergeometric functions, there is an extensive literature dealing with their properties and classification, see for instance [124].

Our focus on discrete measures is because of the application to *Gaussian quadrature* with respect to discrete measures, which is a little known and not yet fully explored spin off of Gaussian quadrature. Quadrature with respect to continuous measures are well-known and go by names such as the Gauss-Hermite quadrature, so we do not explore it here. Some applications will be described in Section 14.3.

But firstly, we are interested in the questions of (re)discovering some orthogonal polynomials. That is, given α , what can we say about the polynomials that are orthogonal with respect to α ? To this end, we follow this simple but effective **procedure**:

- (1) Given α , use Gram-Schmidt orthogonalisation to build up an initial list of polynomials.
- (2) Use this list to guess a recurrence relation of the form (14.24).
- (3) Use the recurrence to determine a generating function for the polynomials.
- (4) Use properties of the recurrence and/or the generating function to prove orthogonality (thus validating the guess).

14.2.1. Charlier polynomials. We demonstrate the procedure above by taking $\alpha = 1/x!$, so we get a sequence of polynomials with

$$\sum_{x=0}^{\infty} \frac{p_n(x)p_m(x)}{x!} = h_n\delta_{nm}.$$

Using Gram-Schmidt, the sequence starts with

$$\begin{aligned} p_1(x) &= x - 1, & p_2(x) &= x^2 - 3x + 1, \\ p_3(x) &= x^3 - 6x^2 + 8x - 1, & p_4(x) &= x^4 - 10x^3 + 29x^2 - 24x + 1. \end{aligned}$$

From the first few p_n , it is not hard to guess that

$$p_n(x) = (x - n)p_{n-1}(x) - (n - 1)p_{n-2}(x), \quad p_{-1}(x) = 0, \quad p_0(x) = 1. \quad (14.26)$$

From (14.26), we shall prove the claimed orthogonality property.

Working with the recursion, it is straightforward to show that the leading coefficient of p_n is 1, and the next coefficient is $-n(n + 1)/2$. Also, $p_n(0) = (-1)^n$, $p_n(1) = (-1)^n(1 - n)$, and $p_n(-1) = (-1)^n e \Gamma(n + 1, 1)$, where $\Gamma(z, a)$ is the incomplete Gamma function (the equality follows as they satisfy the same recurrence). Strong induction gives

$$\begin{aligned} p_n(x + 1) - p_n(x) &= np_{n-1}(x), & (14.27) \\ p_{n+1}(x) + p_n(x) &= xp_n(x - 1). \end{aligned}$$

Armed with these properties, we have

Theorem 14.3 (Orthogonality).

$$\sum_{x=0}^{\infty} \frac{p_n(x)p_m(x)}{x!} = \delta_{nm}n!e. \quad (14.28)$$

PROOF. We only need to consider $\sum_x p_n(x)x^m/x!$ where $m \leq n$. It is easy to check the theorem for small n , so we proceed by induction and assume that the result is true up to $n - 1$. Then, for $p_n(x)$, $\sum_x p_n(x)x^m/x! = 0$ for $m \leq n - 3$ using the recurrences and the inductive hypothesis. Now for $k \in \{1, 2\}$, we have:

$$\begin{aligned} \sum_{x=0}^{\infty} \frac{p_n(x)x^{n-k}}{x!} &= \sum_{x=0}^{\infty} \frac{p_n(x+1)(x+1)^{n-k-1}}{x!} \\ &= \sum_{x=0}^{\infty} \frac{(np_{n-1}(x) + p_n(x))(x+1)^{n-k-1}}{x!} = 0, \end{aligned}$$

where we have used the inductive hypothesis and (14.27). For $k = 0$, we have

$$\sum_{x=0}^{\infty} \frac{p_n(x)x^n}{x!} = \sum_{x=0}^{\infty} \frac{(np_{n-1}(x) + p_n(x))(x+1)^{n-1}}{x!} = n \sum_{x=0}^{\infty} \frac{p_{n-1}(x)x^{n-1}}{x!},$$

by the last equation. Iterating this, and noting $\sum_{x=0}^{\infty} 1/x! = e$, we get $\sum_{x=0}^{\infty} \frac{p_n(x)^2}{x!} = n!e$ as desired. \square

It is easy to show that the exponential generating function for $p_n(x)$ is

$$f(t) = e^{-t}(t+1)^x.$$

This gives another proof of (14.27), and also gives the *umbral* identities

$$p_n(x+y) = \sum_{k=0}^n \binom{n}{k} (-x)_k (-1)^k p_{n-k}(y),$$

$$p'_n(x) = \sum_{k=0}^{n-1} \binom{n}{k} (-1)^{n-k-1} (n-k-1)! p_k(x).$$

Expanding out $f(t)$, we have

$$p_n(x) = (-1)^n {}_2F_0 \left(\begin{matrix} -n, -x \\ - \end{matrix} \middle| -1 \right) = (-1)^n (-x)_n {}_1F_1 \left(\begin{matrix} -n \\ 1-n+x \end{matrix} \middle| 1 \right) = n! L_n^{(x-n)}(1), \quad (14.29)$$

where $L_n^{(a)}(x)$ denotes the generalised Laguerre polynomial. (The symmetry in n and x explains the existence of a partner below (14.27).)

A different generating function is given by

$$\sum_{k=0}^{\infty} \frac{p_n(k)}{k!} x^k = e^x (x-1)^n. \quad (14.30)$$

Setting $x = 1$ in (14.30) and its first $(n-1)$ x -derivatives results in 0 on the right hand side; this gives another proof of orthogonality.

Indeed, what we have rediscovered was a special case (setting $a = 1$ below) of the *Charlier*, or Poisson-Charlier, polynomials, defined by the generating function

$$\sum_{n=0}^{\infty} p_n(x, a) \frac{t^n}{n!} = e^{-t} \left(\frac{t}{a} + 1 \right)^x, \quad (14.31)$$

or by the recurrence

$$a p_n(x, a) = (x - n + 1 - a) p_{n-1}(x, a) - (n-1) p_{n-2}(x, a).$$

Many key properties of the $a = 1$ case are apparent from our analysis. Generalisations of the $a = 1$ case follow readily, for instance we have $p_n(x+1, a) - p_n(x, a) = \frac{n}{a} p_{n-1}(x, a)$ and $p_{n+1}(x, a) + p_n(x, a) = \frac{x}{a} p_n(x-1, a)$. Also,

$$\sum_{x=0}^{\infty} p_n(x, a) \frac{t^x}{x!} = e^t \left(\frac{t}{a} - 1 \right)^n,$$

which gives orthogonality

$$\sum_{x=0}^{\infty} p_m(x, a) p_n(x, a) \frac{a^x}{x!} = \delta_{mn} \frac{n! e^a}{a^n}.$$

Remark 14.2.1 (Connections with Stirling numbers). Writing

$$p_n(x, a) = \sum_{k=0}^n (-1)^k a^{-k} \binom{n}{k} (-x)_k,$$

we see that the coefficient of x^k is

$$\sum_{i=k}^n (-1)^{n-k} a^{-i} \binom{n}{i} \begin{bmatrix} i \\ k \end{bmatrix},$$

here $\begin{bmatrix} n \\ k \end{bmatrix}$ denotes the (unsigned) Stirling numbers of the first kind which satisfies

$$\sum_{k=0}^n \begin{bmatrix} n \\ k \end{bmatrix} x^k = (x)_n.$$

Let $\left\{ \begin{smallmatrix} n \\ k \end{smallmatrix} \right\}$ denote the Stirling numbers of the second kind and let B_n be the n th Bell number; it is well known that

$$\sum_{k=0}^n \left\{ \begin{smallmatrix} n \\ k \end{smallmatrix} \right\} = B_n = \frac{1}{e} \sum_{x=0}^{\infty} \frac{x^n}{x!}.$$

We may then express the orthogonality of $p_n(x, a)$ as a sum involving the Bell numbers and thus Stirling numbers of the second kind. The result is: for integer $0 \leq s \leq n - 1$,

$$\sum_{i,j,k \geq 0} a^{i-k} (-1)^{n-j} \binom{n}{k} \begin{bmatrix} k \\ j \end{bmatrix} \left\{ \begin{smallmatrix} j+s \\ i \end{smallmatrix} \right\} = 0. \tag{14.32}$$

(When $s = n$, the right hand side becomes $n!$.)

Using values for $p_n(\pm 1, a)$, we obtain the (easy) identities

$$\sum_{k=0}^n \sum_{i=k}^n \binom{n}{i} \begin{bmatrix} i \\ k \end{bmatrix} \frac{1}{a^i} = \frac{e^a}{a^n} \Gamma(n+1, a), \quad \sum_{k=0}^n \sum_{i=k}^n \binom{n}{i} \begin{bmatrix} i \\ k \end{bmatrix} \frac{(-1)^k}{a^i} = 1 - \frac{n}{a}.$$

Many more identities may be derived. ◇

Remark 14.2.2 (Two sequences of related polynomials). Let $P_n(x)$ satisfy the recurrence

$$P_n(x) = (x - n - 1)P_{n-1}(x) - (n - 1)P_{n-2}(x),$$

with $P_0(x) = 1, P_1(x) = x - 2$. Favard’s theorem guarantees that P_n is orthogonal with respect to some measure; indeed, the methods outlined in this section give the orthogonality property

$$\sum_{n=1}^{\infty} \frac{P_n(x)P_m(x)}{\Gamma(x)} = \delta_{nm}n!e.$$

The exponential generating function is $e^{-t}(t + 1)^{x-1}$, and $\sum_{k>0} \frac{P_n(k)}{\Gamma(k)} x^k = e^x x(x - 1)^n$.

Clearly, the recurrence bears a resemblance to (14.26). Extracting coefficients, we produce additional identities, for instance

$$\sum_{k=0}^n \sum_{i=k}^n \binom{n}{i} \begin{bmatrix} i \\ k \end{bmatrix} i(-1)^k = -n.$$

We note that [97] computes continuous counterpart to P_n .

Similarly, let $Q_n(x)$ be defined by

$$Q_n(x) = (n - 2 - x)Q_{n-1}(x) + (n - 1)Q_{n-2}(x),$$

with $Q_0(x) = 1, Q_1(x) = -x - 1$. The exponential generating function is $e^{-t}(1 - t)^x$ and $\sum_{k>0} \frac{Q_n(k)}{k!} (-x)^k = e^{-x}(x - 1)^n$. The latter formula leads to

$$\sum_{n=0}^{\infty} Q_n(x)Q_m(x) \frac{(-1)^x}{x!} = \delta_{nm} \frac{(-1)^n n!}{e},$$

so Q_n is the alternating analog of p_n . Looking at $Q_n(1)$, we get the identity

$$\sum_{k=0}^n \sum_{i=k}^n \binom{n}{i} \begin{bmatrix} i \\ k \end{bmatrix} (-1)^{i+k} = 1 + n.$$

Note that by trying different weights, we may *rule out* the existence of polynomials with nice recurrences, generating functions or closed forms for many α (c. f. a similar philosophy is used in Chapter 13). ◊

14.2.2. Meixner polynomials. Taking $\alpha = 1/2^x$, we produce a sequence of orthogonal polynomials which seems to satisfy the recursion

$$n m_n(x) = (x - 3n + 2)m_{n-1}(x) - 2(n - 1)m_{n-2}(x), \quad m_{-1}(x) = 0, \quad m_0(x) = 1.$$

We will now show that $m_n(x)$ defined by this recursion are indeed orthogonal with respect to α . It is standard to find the generating function

$$\sum_{n=0}^{\infty} m_n(x)t^n = \frac{(2t + 1)^x}{(t + 1)^{x+1}},$$

from which it follows that

$$m_n(x+1) - m_n(x) = \sum_{k=0}^{n-1} (-1)^{n-k-1} m_k(x). \quad (14.33)$$

We are ready to prove:

Theorem 14.4 (Orthogonality).

$$\sum_{x=0}^{\infty} \frac{m_n(x)m_m(x)}{2^x} = \delta_{mn}2^{n+1}.$$

PROOF. For ease of notation we denote the sum above as an inner product. We proceed by induction. The statement is true for small $m \leq n$; assume orthogonality is true up to m_{n-1} (though for $m = n-1$ we may not know the explicit right hand side). Then, appealing to the recursion, we may deduce that $\langle m_m, m_m \rangle = 2^{m+1}$ for $m \leq n-2$, and $\langle m_n, m_m \rangle = 0$ for $m \leq n-3$. We are left to find the values of $\langle m_n, m_{n-2} \rangle$, $\langle m_{n-1}, m_{n-1} \rangle$ and $\langle m_n, m_{n-1} \rangle$.

For the first inner product, we have

$$\sum_{x=0}^{\infty} \frac{m_n(x)m_{n-2}(x)}{2^x} = 1 + \frac{1}{2} \sum_{x=0}^{\infty} \frac{m_n(x+1)m_{n-2}(x+1)}{2^x}.$$

Now we expand the right hand side by (14.33) while denoting the left hand side by S :

$$\begin{aligned} S &= 1 + \frac{1}{2} \sum_{x=0}^{\infty} \{2^{-x}(m_n(x) + m_{n-1}(x) - m_{n-2}(x) + m_{n-3}(x) - \cdots) \\ &\quad \times (m_{n-2}(x) + m_{n-3}(x) - m_{n-4}(x) + m_{n-5}(x) - \cdots)\} \\ &= 1 + \frac{1}{2}S + \frac{1}{2}(-\langle m_{n-2}, m_{n-2} \rangle + \langle m_{n-3}, m_{n-3} \rangle + \langle m_{n-4}, m_{n-4} \rangle + \cdots) \\ &= 1 + \frac{1}{2}S + \frac{1}{2}(-2^{n-1} + 2^{n-2} + 2^{n-3} + \cdots + 2) = \frac{1}{2}S, \end{aligned}$$

so $S = 0$. This also establishes, via the recursion, that $\langle m_{n-1}, m_{n-1} \rangle = 2^n$.

It remains to show that $\langle m_n, m_{n-1} \rangle = 0$. Proceeding as before, we denote the sum by T :

$$\begin{aligned}
T &= -1 + \frac{1}{2} \sum_{x=0}^{\infty} \frac{m_n(x+1)m_{n-1}(x+1)}{2^x} \\
&= -1 + \frac{1}{2} \sum_{x=0}^{\infty} \{2^{-x}(m_n(x) + m_{n-1}(x) - m_{n-2}(x) + m_{n-3}(x) - \dots) \\
&\quad \times (m_{n-1}(x) + m_{n-2}(x) - m_{n-3}(x) + m_{n-4}(x) - \dots)\} \\
&= -1 + \frac{1}{2}T + \frac{1}{2}(\langle m_{n-1}, m_{n-1} \rangle - \langle m_{n-2}, m_{n-2} \rangle - \langle m_{n-3}, m_{n-3} \rangle + \dots) \\
&= -1 + \frac{1}{2}T + \frac{1}{2}(2^n - 2^{n-1} - 2^{n-2} - \dots - 2) = -1 + \frac{1}{2}T + \frac{1}{2}(2^n - 2^n + 2),
\end{aligned}$$

Thus $T = 0$. The inductive step is complete. \square

In fact, we just rediscovered a very special case of the *Meixner* polynomials, $M_n(x, b, c)$ (with $b = 1$, $c = 1/2$), which may be defined by the ordinary generating function $\frac{(1-t/c)^x}{(1-t)^{x+b}}$. In hypergeometric terms, it is

$$M_n(x, b, c) = \frac{(b)_n}{n!} {}_2F_1 \left(\begin{matrix} -n, -x \\ b \end{matrix} \middle| 1 - \frac{1}{c} \right). \quad (14.34)$$

A recurrence for M_n can be found using *contiguous* relations (Section 14.1); indeed, denoting the ${}_2F_1$ part by $m_n(x, b, c)$, we have

$$c(n+b)m_{n+1}(x) = ((c-1)x + (n+nc+bc))m_n(x) - nm_{n-1}(x), \quad (14.35)$$

and due to symmetry we get another relation with the roles of x and n interchanged.

The general orthogonality property is

$$\sum_{x \geq 0} M_n(x)M_m(x) \frac{(b)_x c^x}{x!} = \delta_{mn} \frac{(b)_n c^{-n}}{n!(1-c)^b}. \quad (14.36)$$

For $b = 1$, the proof of orthogonality can be easily adapted from the proof of Theorem 14.4. For other positive integer b , a proof follows readily by induction and the contiguous relation

$$c(n+1)M_{n+1}(x, b, c) = (n+b)M_n(x, b, c) + (b+x)(c-1)M_n(x, b+1, c).$$

Thus, we have recaptured several properties of the Meixner polynomials using mostly elementary analysis and generating functions, without resorting to advanced theory.

Remark 14.2.3. Using the ${}_2F_1$ representation, we see that the coefficient of x^k in $m_n(x)$ is

$$\sum_{i=k}^n \frac{(-1)^k}{i!} \binom{n}{i} \begin{bmatrix} i \\ k \end{bmatrix},$$

and $m_n(n)$ has the closed form $(-1)^{n/2} \binom{n}{n/2}$ when n is even, and 0 otherwise.

It is also easy to show that a closely related sequence, given by $m'_n(x) = {}_2F_1(-n, 1-x, 2, -1)$, satisfies

$$\sum_{x=0}^{\infty} m'_n(x) m'_m(x) \frac{x}{2^x} = \delta_{mn} \frac{2^{n+1}}{n+1}.$$

A connection between the Meixner and the Charlier polynomials is given by

$$\lim_{b \rightarrow \infty} m_n\left(x, b, \frac{a}{a+b}\right) = p_n(x, a).$$

◇

14.3. Gaussian quadrature

The classical theory of Gaussian quadrature is a scheme for approximating integrals by finite sums involving orthogonal polynomials (see [11, Ch. 5]). More specifically, in the notation of (14.23) and (14.24), and using $d\alpha = \omega(x)dx$, we have

Proposition 14.1 (Gaussian quadrature).

$$\int_a^b f(x) \omega(x) dx = \sum_{i=1}^n f(x_i) w_i + R_n, \quad (14.37)$$

where x_i are the roots of $p_n(x)$, w_i are the weights defined by

$$w_i = \frac{-h_n}{p_{n+1}(x_i) p'_n(x_i)}, \quad (14.38)$$

and R_n is the error which depends on the $(2n)$ th derivative of f . In particular, if f is a polynomial of degree $\leq 2n-1$, $R_n = 0$ and the quadrature is exact.

Note that by its very construction (i. e. the usage of roots), Gaussian quadrature is exact for polynomials of degree up to $n-1$; orthogonality gives exactness for higher degrees, and it is this pleasing property which makes Gaussian quadrature superior to many other schemes. In practice, the error is difficult to compute, and is best estimated on a case-by-case basis by fixing f and increasing n . Heuristically, if f is closely approximated by polynomials on (a, b) (e. g. if it has a close-fitting Taylor series), then Gaussian quadrature tends to work well; this implies that given an

integrand, we need to choose the weight ω carefully – for instance to cancel out any singularities.

In practice, the Legendre and Chebyshev polynomials are often used for Gaussian quadrature, which means $a = -b = 1$. In order to perform quadrature for an integral over $(0, \infty)$, the transformation $x \mapsto (1 - x)/(1 + x)$ can be used.

Engblom [90] was one of the first to give a comprehensive report on Gaussian quadrature using discrete measures. He noted that the classical theory carried over exactly if α were discrete, that is, one would have

$$\sum_x f(x)\alpha(x) \approx \sum_{i=1}^n f(x_i)w_i. \quad (14.39)$$

Engblom demonstrated his concepts by using the Charlier and Meixner polynomials to numerically compute hypergeometric functions.

Example 14.3.1. Monien [151], using reciprocal polynomials, considered orthogonal conditions of the form

$$\sum_{x>0} f_n\left(\frac{1}{x^2}\right)f_m\left(\frac{1}{x^2}\right)\frac{1}{x^2} = h_n\delta_{mn}.$$

By looking at the continued fraction of the moment generating function, Monien derives a recurrence for $f_n(x)$ which takes a particularly simple form in terms of Bessel functions. Quadrature using f_n works particularly well for summands $f(x)$ which admit an asymptotic expansion in powers of $1/x^2$ for large x . For instance, Monien used it fruitfully for the Hardy-Littlewood sum $\sum_{x>0} \sin(a/x)/x$, traditionally considered challenging computationally for large a . The procedure works the same way as before: one computes the roots x_i of $f_n(x)$, from which w_i follows. Since $f_n(1/x^2)$ is used instead, the right hand side of (14.39) needs to be replaced by $\sum_{i=1}^n f(1/\sqrt{x_i})w_i$. \diamond

The following **procedure** can be used for Gaussian quadrature on sums: Given some α , it is easy to generate a table of orthogonal polynomials (Gram-Schmidt). We may then find the roots using say Newton's method (when the table is small), or by exploiting the fact that the zeros are eigenvalues of a tridiagonal matrix, and stable, fast algorithms exist for finding them. The weights can then be computed, either using (14.38), or by exploiting the fact that Gaussian quadrature is exact for low degree elementary polynomials (whose sums involving the weights can be found

independently). This way finding w_i is equivalent to inverting a Vandermonde matrix whose columns are powers of r_i (the explicit inverse is given in terms of Stirling numbers [137]). Once a reasonably large table has been computed (to say a few thousand digits), it can be reused for similar sums.

In the following table, we have recorded the results of a number of discrete Gaussian quadrature on non-trivial sums, with varying orthogonal polynomials, *numbers of weights* (n), and numbers of *correct digits* obtained, to indicate that a range of sums may be approximated to different levels of desired accuracy.

orthogonality	poly.	summand	n	digits	comment
$\sum_x f_n(\frac{1}{x^2})f_m(\frac{1}{x^2})\frac{1}{x^2}$	Monien	$\frac{\sin(\frac{10^4}{x})}{x}$	150	167	Hardy-Littlewood
$\sum_x f_n(\frac{1}{x^2})f_m(\frac{1}{x^2})\frac{1}{x^3}$		$\frac{\cos(\frac{1}{x})-1}{x}$	15	50	
$\sum_x f_n(\frac{1}{x})f_m(\frac{1}{x})\frac{1}{x^2}$		$\frac{1}{x} - \ln \frac{x+1}{x}$	20	54	Euler γ
$\sum_x p_n(x)p_m(x)\frac{1}{x!}$	Charlier	$\frac{\exp(\sin x)}{x!}$	30	20	
$\sum_x p_n(x)p_m(x)\frac{1}{2^x}$	Meixner	$\frac{I_0(x/4)}{2^x}$	50	67	

For example, with the second entry in the table, we chose that particular orthogonality condition because the asymptotic expansion of the summand at infinity contains only odd powers of x . For better behaved sums, Gaussian quadrature is very powerful, for instance, using $n = 50$, $\sum_x 1/(x^2 + 1) = \pi \coth \pi$ may be approximated to 282 digits.

14.3.1. Lattice sums. Lattice sums, as the name implies, are multi-dimensional sums over lattices and often hold chemical importance, for instance they may be used to determine the electrostatic potential of an ion in a crystal. A comprehensive guide can be found in [102] (which is expanded in [52]). We observe that Gaussian quadrature can be applied to approximate lattice sums.

We start with the Hardy-Lorenz sum [205],

$$\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty}{}' \frac{1}{(m^2 + n^2)^s} = 4\beta(s)\zeta(s). \quad (14.40)$$

The prime denotes that the $m = n = 0$ term is to be omitted, and $\beta(s)$ denotes the Dirichlet beta function, see Chapter 13. As a proof of concept, consider the $s = 2$ case (where the exact answer is $2G\pi^2/3$). We can in fact perform one summation exactly, since

$$\sum_{n=-\infty}^{\infty} \frac{1}{m^2 + n^2} = \frac{\pi}{m} \coth(m\pi),$$

and we then take the derivative of both sides with respect to m . The resulting sum (replacing m by x) behaves like $\pi/(4x^3) - 1/(2x^4)$ for large x , so the polynomials f_n with orthogonality conditions

$$\sum_x f_n\left(\frac{1}{x}\right) f_m\left(\frac{1}{x}\right) \frac{1}{x^2} = \delta_{mn} h_n \quad (14.41)$$

should be used for quadrature. Using only 20 weights, we obtain 31 correct digits. (With the right implementation, Gram-Schmidt is very fast at computing f_n , therefore obtaining hundreds of weights is computationally cheap.)

For many lattice sums, it is not possible to perform one summation explicitly; also, many sums are alternating. Our next example will tackle both of these problems. Consider the sum

$$S = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} ' \frac{(-1)^{m+n}}{(m^2 + n^2)^2}.$$

For Gaussian quadrature, we use the polynomials g_n with orthogonality conditions

$$\sum_x g_n\left(\frac{1}{x}\right) g_m\left(\frac{1}{x}\right) \frac{(-1)^x}{x} = \delta_{mn} h_n.$$

We perform a double quadrature on S , that is, we first perform quadrature on $f(n) = mn/(m^2 + n^2)^2$ (since the weight is $(-1)^n/n$). This gives a finite sum of functions of m , which we perform quadrature upon as our new function. Using only 10 weights, this method gives 15 correct digits.

In our investigation in Chapter 7, the lattice sum (7.52) was first verified to 53 digits using Gaussian quadrature with 50 weights, which convinced us of its veracity and gave us impetus to find a proof.

Many lattices sums, including higher-dimensional ones such as the classical *Madelung constant* [42],

$$M = \sum_{n,m,p} ' \frac{(-1)^{n+m+p}}{\sqrt{n^2 + m^2 + p^2}},$$

may be approximated using the scheme described here. We obtain 36 digits for M using only 25 weights; roughly 1.4 extra digits are obtained for each additional weight. It is interesting to note that the sum for M converges very slowly, and naïve approaches struggle to obtain even 2 or 3 digits of accuracy.

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