Random Walks, Elliptic Integrals and Related Constants

James Gu feng Wan

BSc (Hons)

Dissertation Submitted To
The School of Mathematical and Physical Sciences
At The University of Newcastle
For the Degree of
Doctor of Philosophy (Mathematics)

Submitted: March 2013 Revised: July 2013
**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.

Candidate name: _______________  Candidate signature: _______________  

**Statement of Collaboration**

I hereby certify that the work embodied in this thesis has been done in collaboration with other researchers. I have included as part of the thesis a statement clearly outlining the extent of collaboration, with whom and under what auspices.

**Statement of Authorship**

I hereby certify that the work embodied in this thesis contains published papers/scholarly work of which I am a joint author. I have included as part of the thesis a written statement, endorsed by my supervisor, attesting to my contribution to the joint publications/scholarly work.

Candidate signature: _______________  Date: _______________
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 They have not appeared in print, except: Section 7.9 is a paraphrasing of my unpublished joint article [169], Section 8.4 comes from my contribution to the published joint paper [41], Section 12.5 has been placed on-line [191], and a brief summary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
I declare that the details provided above are correct.

Candidate Signature: ________________

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
### CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.2</td>
<td>Three-step walk with different step lengths</td>
<td>69</td>
</tr>
<tr>
<td>4.3</td>
<td>Higher dimensions</td>
<td>71</td>
</tr>
<tr>
<td>4.4</td>
<td>Limiting the number of directions</td>
<td>77</td>
</tr>
<tr>
<td></td>
<td>Chapter 5. Moments of Elliptic Integrals and Catalan’s Constant</td>
<td></td>
</tr>
<tr>
<td>5.1</td>
<td>Introduction and background</td>
<td>79</td>
</tr>
<tr>
<td>5.2</td>
<td>Basic results</td>
<td>82</td>
</tr>
<tr>
<td>5.3</td>
<td>Closed form initial values</td>
<td>88</td>
</tr>
<tr>
<td>5.4</td>
<td>Contour integrals for $G_s$</td>
<td>91</td>
</tr>
<tr>
<td>5.5</td>
<td>Closed forms at negative integers</td>
<td>92</td>
</tr>
<tr>
<td></td>
<td>Chapter 6. Moments of Products of Elliptic Integrals</td>
<td></td>
</tr>
<tr>
<td>6.1</td>
<td>Motivation and general approach</td>
<td>95</td>
</tr>
<tr>
<td>6.2</td>
<td>One elliptic integral</td>
<td>97</td>
</tr>
<tr>
<td>6.3</td>
<td>Two complementary elliptic integrals</td>
<td>98</td>
</tr>
<tr>
<td>6.4</td>
<td>One elliptic integral and one complementary elliptic integral</td>
<td>102</td>
</tr>
<tr>
<td>6.5</td>
<td>Sporadic results</td>
<td>105</td>
</tr>
<tr>
<td>6.6</td>
<td>Fourier series</td>
<td>107</td>
</tr>
<tr>
<td>6.7</td>
<td>Legendre’s relation</td>
<td>109</td>
</tr>
<tr>
<td>6.8</td>
<td>Integration by parts</td>
<td>110</td>
</tr>
<tr>
<td></td>
<td>Chapter 7. More Integrals of $K$ and $E$</td>
<td></td>
</tr>
<tr>
<td>7.1</td>
<td>One elliptic and one complementary elliptic integral</td>
<td>119</td>
</tr>
<tr>
<td>7.2</td>
<td>Two complementary elliptic integrals</td>
<td>122</td>
</tr>
<tr>
<td>7.3</td>
<td>Two elliptic integrals</td>
<td>123</td>
</tr>
<tr>
<td>7.4</td>
<td>More on explicit primitives</td>
<td>125</td>
</tr>
<tr>
<td>7.5</td>
<td>Some other integrals</td>
<td>126</td>
</tr>
<tr>
<td>7.6</td>
<td>Incomplete moments</td>
<td>129</td>
</tr>
<tr>
<td>7.7</td>
<td>One elliptic integral with parameters</td>
<td>130</td>
</tr>
<tr>
<td>7.8</td>
<td>Fourier series and three elliptic integrals</td>
<td>132</td>
</tr>
<tr>
<td>7.9</td>
<td>Proof of the conjecture</td>
<td>134</td>
</tr>
<tr>
<td>7.10</td>
<td>Some hypergeometric identities</td>
<td>138</td>
</tr>
<tr>
<td></td>
<td>Chapter 8. Elementary Evaluations of Mahler Measures</td>
<td></td>
</tr>
<tr>
<td>8.1</td>
<td>Jensen’s formula and Mahler measures</td>
<td>141</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>---------</td>
<td>----------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>8.2</td>
<td>On $\mu(k + x + 1/x + y + 1/y)$</td>
<td>148</td>
</tr>
<tr>
<td>8.3</td>
<td>On $\mu((1 + x)(1 + y) + z)$</td>
<td>150</td>
</tr>
<tr>
<td>8.4</td>
<td>Proofs of two conjectures of Boyd</td>
<td>151</td>
</tr>
<tr>
<td>9.1</td>
<td>Introduction</td>
<td>155</td>
</tr>
<tr>
<td>9.2</td>
<td>Preliminaries and log-sine integrals</td>
<td>156</td>
</tr>
<tr>
<td>9.3</td>
<td>Mahler measures and moments of random walks</td>
<td>160</td>
</tr>
<tr>
<td>9.4</td>
<td>Epsilon expansion of $W_3$</td>
<td>161</td>
</tr>
<tr>
<td>9.5</td>
<td>Trigonometric analysis of $\mu_n(1 + x + y)$</td>
<td>164</td>
</tr>
<tr>
<td>9.6</td>
<td>Evaluation of $\mu_2(1 + x + y)$</td>
<td>172</td>
</tr>
<tr>
<td>10.1</td>
<td>Introduction</td>
<td>175</td>
</tr>
<tr>
<td>10.2</td>
<td>Brafman’s formula and modular equations</td>
<td>176</td>
</tr>
<tr>
<td>10.3</td>
<td>Identities for $s = 1/2$</td>
<td>181</td>
</tr>
<tr>
<td>10.4</td>
<td>Identities for $s = 1/3$</td>
<td>184</td>
</tr>
<tr>
<td>10.5</td>
<td>Identities for $s = 1/4$</td>
<td>187</td>
</tr>
<tr>
<td>10.6</td>
<td>New identities for $s = 1/6$</td>
<td>191</td>
</tr>
<tr>
<td>10.7</td>
<td>Companion series</td>
<td>192</td>
</tr>
<tr>
<td>10.8</td>
<td>Closed forms</td>
<td>193</td>
</tr>
<tr>
<td>10.9</td>
<td>Summary</td>
<td>194</td>
</tr>
<tr>
<td>10.10</td>
<td>Complex Series for $1/\pi$</td>
<td>195</td>
</tr>
<tr>
<td>11.1</td>
<td>Introduction</td>
<td>203</td>
</tr>
<tr>
<td>11.2</td>
<td>Apéry-like sequences</td>
<td>206</td>
</tr>
<tr>
<td>11.3</td>
<td>Generalised Bailey’s identity</td>
<td>209</td>
</tr>
<tr>
<td>11.4</td>
<td>Generating functions of Legendre polynomials</td>
<td>210</td>
</tr>
<tr>
<td>11.5</td>
<td>Formulas for $1/\pi$</td>
<td>212</td>
</tr>
<tr>
<td>11.6</td>
<td>Concluding remarks</td>
<td>218</td>
</tr>
<tr>
<td>12.1</td>
<td>Orthogonal polynomials</td>
<td>221</td>
</tr>
<tr>
<td>12.2</td>
<td>Orr-type theorems and contiguous relations</td>
<td>224</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>---------</td>
<td>-------</td>
<td>------</td>
</tr>
<tr>
<td>12.3.</td>
<td>A miscellany of results on $\pi$</td>
<td>228</td>
</tr>
<tr>
<td>12.4.</td>
<td>New generating functions</td>
<td>233</td>
</tr>
<tr>
<td>12.5.</td>
<td>Series for $1/\pi$ using Legendre’s relation</td>
<td>238</td>
</tr>
</tbody>
</table>

Chapter 13. Weighted Sum Formulas for Multiple Zeta Values 253

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.1.</td>
<td>Introduction</td>
<td>253</td>
</tr>
<tr>
<td>13.2.</td>
<td>Elementary proofs</td>
<td>254</td>
</tr>
<tr>
<td>13.3.</td>
<td>New sums</td>
<td>256</td>
</tr>
<tr>
<td>13.4.</td>
<td>More sums from recursions</td>
<td>265</td>
</tr>
<tr>
<td>13.5.</td>
<td>Length 3 and higher multiple zeta values</td>
<td>272</td>
</tr>
<tr>
<td>13.6.</td>
<td>Another proof of Zagier’s identity</td>
<td>279</td>
</tr>
</tbody>
</table>

Chapter 14. Further Applications of Experimental Mathematics 283

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>14.1.</td>
<td>Contiguous relations</td>
<td>283</td>
</tr>
<tr>
<td>14.2.</td>
<td>Orthogonal polynomials</td>
<td>293</td>
</tr>
<tr>
<td>14.3.</td>
<td>Gaussian quadrature</td>
<td>301</td>
</tr>
</tbody>
</table>

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. INTRODUCTION

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],


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],


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],

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],

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],
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],

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


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],


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],

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],


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 \cite{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,

$$\displaystyle pF_q \left( \begin{array}{c} a_1, \ldots, a_p \\ b_1, \ldots, b_q \end{array} \bigg| z \right) = \sum_{n=0}^{\infty} \frac{(a_1)_n \cdots (a_p)_n \ z^n}{(b_1)_n \cdots (b_q)_n \ n!},$$

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 written in terms of hypergeometric series and well-known constants (such as $\pi$).

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

$$K(x) = \frac{\pi}{2} \, 2F_1 \left( \begin{array}{c} \frac{1}{2}, 1 \\ 1 \end{array} \bigg| x^2 \right) = \int_0^{\pi/2} \frac{dt}{\sqrt{1 - x^2 \sin^2 t}},$$

$$E(x) = \frac{\pi}{2} \, 2F_1 \left( \begin{array}{c} -\frac{1}{2}, \frac{1}{2} \\ 1 \end{array} \bigg| x^2 \right) = \int_0^{\pi/2} \frac{\sqrt{1 - x^2 \sin^2 t} \ dt}{\sqrt{1 - x^2 \sin^2 t}}.$$

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].
0.2. OVERVIEW

The Riemann zeta function is given, for $\text{Re } s > 1$, 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 $\approx$.

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

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

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

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

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

$$W_{2n}(s) \approx \sum_{j \geq 0} \binom{s/2}{j}^2 W_{2n-1}(s - 2j), \quad (0.3)$$
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
\[
p_2(x) = \frac{2}{\pi \sqrt{4 - x^2}}, \quad W_2(s) = \binom{s}{s/2}, \tag{0.4}
\]
a closed form formula for \( W_3(s) \) involves more effort. Our result is in terms of the generalised hypergeometric series: for integer \( k \),
\[
W_3(k) = \text{Re} \, _3F_2 \left( \frac{1}{2}, -\frac{k}{2}, -\frac{k}{2} \middle| \frac{1}{4} \right). \tag{0.5}
\]
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,
\[
W_3(1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6 \left( \frac{1}{3} \right) + \frac{27}{4} \frac{2^{2/3}}{\pi^4} \Gamma^6 \left( \frac{2}{3} \right), \tag{0.6}
\]
as well as
\[
W_3(-1) = \frac{3}{16} \frac{2^{1/3}}{\pi^4} \Gamma^6 \left( \frac{1}{3} \right). \tag{0.7}
\]

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
\[
W_4(-1) = \frac{\pi}{4} \, _7F_6 \left( \frac{5}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| 1, 1, 1, 1, 1, 1 \right), \tag{0.8}
\]
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
\[
W_4(-1) = \frac{8}{\pi^3} \int_0^1 K^2(k) \, dk = \frac{4}{\pi^3} \int_0^1 K''(k)^2 \, dk. \tag{0.9}
\]
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

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

\[ p_4(x) = \frac{2}{\pi^2} \frac{\sqrt{16 - x^2}}{x} \text{Re} _3F_2\left( \frac{1}{5}, \frac{1}{6}; \frac{1}{7}; \frac{(16 - x^2)^3}{108x^4} \right). \quad (0.11) \]

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 \(-1\):

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

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 \( s \):

\[ W_4(s) = \frac{2^{2s+1}}{\pi^2 \Gamma(\frac{1}{2}(s + 2))^2} G_{2,4}^{4,4}\left( \frac{1, 1, \frac{s+3}{2}, \frac{s+2}{2}, \frac{s+2}{2}, \frac{1}{2}}{\frac{s+2}{2}, \frac{s+2}{2}, \frac{s+2}{2}, \frac{1}{2}} ; \frac{1}{4} \right). \quad (0.13) \]

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 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 \( \frac{4\pi}{\Gamma(1/4)^2} + \frac{\Gamma(1/4)^4}{4\pi^3} \). 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 $K^*$ and $E^*$. 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 $\, _2F_1$ 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 $\pi$ and $\pi^3$. 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:

\[
\int_{0}^{1} \left( \frac{x}{\sqrt{x}} \right)^{\frac{1}{2} \pm \frac{1}{4}} K(x) \, dx = \frac{\pi^2}{12} \sqrt{5 \pm \frac{1}{\sqrt{2}}}. 
\]

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

\[
\int_{0}^{1} K'(x)^3 \, dx = 3 \int_{0}^{1} K(x)^2 K'(x) \, dx = 5 \int_{0}^{1} x K'(x)^3 \, dx = \frac{\Gamma^8(1/4)}{128\pi^2}. 
\] (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 \( W_4'(0) = \frac{7}{2} \frac{\zeta(3)}{\pi^3} \) (here \( \text{Cl} \) 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

\[
\mu(P_1, P_2, \ldots, P_k) := \int_{0}^{1} \cdots \int_{0}^{1} \prod_{j=1}^{k} \log |P_j(e^{2\pi it_1}, \ldots, e^{2\pi it_n})| \, dt_1 dt_2 \cdots dt_n.
\]

The connection with random walks is that

\[
W_n^{(m)}(0) = \mu_m(1 + x_1 + \ldots + x_{n-1}).
\]
where \( \mu_m(P) = \mu(P, \ldots, P) \) 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:

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

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

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

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

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

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

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

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,

$$\sum_{n=0}^{\infty} \frac{(s)_n(1-s)_n}{n!^2} P_n(x) z^n = 2F_1\left(s, \frac{1-s}{2} \begin{array}{c} \frac{1}{2} \end{array} \; \begin{array}{c} 1 - \rho - z \end{array} \; \begin{array}{c} 1 - \rho + z \end{array} \right),$$

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 $\alpha$ and $\beta$ 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,

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

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

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

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,
\[
\sum_{n=0}^{\infty} u_n P_n \left( \frac{(X + Y)(1 + cXY) - 2aXY}{(Y - X)(1 - cXY)} \right) \left( \frac{Y - X}{1 - cXY} \right)^n
= (1 - cXY) \left\{ \sum_{n=0}^{\infty} u_n X^n \right\} \left\{ \sum_{n=0}^{\infty} u_n Y^n \right\},
\]
(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
\[
\sum_{n=0}^{\infty} \left( \frac{1}{2} \right)^n \left( \frac{1}{n!} \right)^2 P_{2n} \left( \frac{(X + Y)(1 - XY)}{(X - Y)(1 + XY)} \right) \left( \frac{X - Y}{1 + XY} \right)^{2n}
= \frac{1 + XY}{2} {}_2F_1 \left( \frac{1}{2}, \frac{1}{2} \bigg| 1 - X^2 \right) {}_2F_1 \left( \frac{1}{2}, \frac{1}{2} \bigg| 1 - Y^2 \right).
\]
(0.19)

We are thus able to find new series for $1/\pi$ whose summands involve Apéry-like sequences or rarefied Legendre polynomials, examples of which include
\[
\sum_{n=0}^{\infty} \left( \frac{1}{2} \right)^n \left( \frac{1}{n!} \right)^2 P_{2n} \left( \frac{3\sqrt{3}}{5} \right) \left( \frac{2\sqrt{2}}{5} \right)^{2n} = \frac{15}{\pi},
\]
\[
\sum_{n=0}^{\infty} \left( \frac{1}{3} \right)^n \left( \frac{4}{n!} \right)^3 P_{3n} \left( \frac{4}{\sqrt{10}} \right) \left( \frac{1}{\sqrt{10}} \right)^{3n} = \frac{\sqrt{15 + 10\sqrt{3}}}{\pi \sqrt{2}},
\]
\[
\sum_{n=0}^{\infty} \left\{ \sum_{k=0}^{n} \sum_{j=0}^{k} \left( \frac{n}{k} \right) \left( \frac{-1}{8} \right)^k \left( \frac{k}{j} \right)^3 \right\} n P_n \left( \frac{5}{3\sqrt{3}} \right) \left( \frac{4}{3\sqrt{3}} \right)^n = \frac{9\sqrt{3}}{2\pi}.
\]

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
\[
\sum_{n=0}^{\infty} \sum_{k=0}^{n} \binom{2n-2k}{n-k} \binom{2k}{k} \binom{2n}{n} \frac{x^{k+n}}{(1+4x)^{2n+1}} = 3F_2 \left( \frac{1}{3}, \frac{1}{2}; \frac{2}{3} \middle| \frac{1}{1}, 1 \right) 108x^2(1-4x),
\]
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
\[
\sum_{n=0}^{\infty} \frac{1}{n!^3} \frac{1}{n\left( \frac{5}{6} \right)_n} \left( \frac{1}{125} \right)^n (1+11n) = \frac{5\sqrt{15}}{6\pi},
\]
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,
\[
\sum_{j=2}^{s-1} 2^j \zeta(j, s-j) = (s+1)\zeta(s),
\]
as discover its alternating companion,
\[
\sum_{j=2}^{s-1} 2^j \zeta(j, s-j) = (3 - 2^{2-s} - s)\zeta(s).
\]
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 $H_n$,

$$
\sum_{n=0}^{\infty} \frac{H_n}{(2n + 1)^{2s-1}} = (1 - 4^{-s})(2s - 1)\zeta(2s) - (2 - 4^{1-s}) \log(2)\zeta(2s - 1)
$$

$$
+ (1 - 2^{-s})^2 \zeta(s)^2 - \sum_{k=2}^{s} 2(1 - 2^{-k})(1 - 2^{k-2s})\zeta(k)\zeta(2s - k).
$$

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

$$
\sum_{j=2}^{n-2} (j - 1)(2j - 1)(n - j - 1)(2n - 2j - 1)\zeta(2j, 2n - 2j) = \frac{3}{8}(n - 1)(3n - 2)\zeta(2n) - 3(2n - 5)\zeta(4)\zeta(2n - 4).
$$

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 $\zeta$ convolution identity which was first discovered experimentally. Results such as the above, where the right hand side is a rational multiple of $\pi^{2n}$, 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.